

A Macro-scale, Tribological Modeling Framework
for Simulating Multiple Lubrication Regimes and
Engineering Applications

Gagan Srivastava

Ph.D. Candidate
Mechanical Engineering Department
Carnegie Mellon University

Abstract

Tribology is the science of interacting surfaces and the associated study of friction lubrication and wear. High friction and wear cause energy loss and deterioration of interacting surfaces. Lubrication, using hydrodynamic liquids is the primary mechanism to reduce friction and wear. Unfortunately, not all applications can be ideally lubricated to operate in a low friction zone. In the majority of cases, the relative velocities between the moving components is either too low, or the transferred force is too high for them to get perfectly lubricated, with minimal solid to solid contact. In such conditions they operate in the boundary or mixed lubrication regime, where there is significant solid-solid contact. Examples of such conditions are commonplace in our daily lives. From the food in our mouth to a floating hard disk drive read/write heads, or artificial hip joints to a polishing process, all operate in the mixed lubrication regime.

In this thesis, a generalized numerical modeling framework has been developed that can be applied to simulate the operation of a large variety tribological applications that operate in any of the three lubrication regimes. The framework called the *Particle Augmented Mixed Lubrication - Plus* (PAML+), accounts for all the major mechanical interactions encountered in any tribosystem. It involves coupled

modules for solid mechanics and fluid mechanics. Depending on the application, additional fidelity has been added in the form of modules relevant to the physical interactions unique to the application. For example, modeling of the chemical mechanical polishing process requires treatment of particle dynamics and wear to be able to generate predictions of meaningful quantities such as the material removal rate. Similarly, modeling of artificial hip joints requires additional treatment of mass transport and wear to simulate contamination with debris particles.

The fluid mechanics have been modeled through the thin film approximation of Navier Stokes equations, known as the Reynolds Equation. The solid mechanics have been modeled using analytical or semi-analytical techniques. Statistical treatments have been applied to model particle dynamics wherever required to avoid huge computational requirements associated with deterministic methods such as the discrete element method.

To demonstrate the strengths and general applicability of the modeling approach, four major tribological applications have been modeled using the new modeling approach in order to broadly impact key industries. The four tribological applications are (i) Pin-on-disk tribosystems (ii) Chemical mechanical polishing (CMP) (iii) Artificial hip joints, and (iv) Mechanical seals. First the model was employed to simulate pin-on-disk interfaces to evaluate different surface texture designs. It also served as a platform to test the model's ability to capture, and seamlessly traverse through different lubrication regimes. The model predicted that an intermediate texture dimension of $200\mu\text{m}$ resulted in 80% lesser wear than a larger texture of $200\mu\text{m}$, and up to 90% lesser wear than an untextured sample. Second, the framework was employed to study the CMP process. Overall, the model was found to be at least 50% more accurate than the previous generation model. Third, the model

was tailored to study the artificial joints. Wear predictions from the model remained within 5% error upon comparing against the experiments, while studying different “head” sizes. It was discovered that textured joints can reduce the concentration of the wear debris by at least 2.5% per cycle. For an expected lifetime of 12 years, that translates to lifetime enhancement of 3 months. Lastly, the model was employed to study the performance of mechanical seals. Even though the model was much more computationally efficient, it remained within 5% of much more detailed and computationally expensive FEA models. The model also predicted that the seals allow the highest leakage at shaft speeds of about 950 RPM.

Acknowledgements

I would like to thank my research advisor Prof. C. Fred Higgs III for his guidance throughout my PhD. I am grateful to him for trusting me with the responsibility of tackling difficult industrial problems, and representing the Particle Flow and Tribology Laboratory (PFTL) in front of important customers. I am specially thankful for his advice on and off the lab, that not only guided me through difficult times in my research, but would also become a key factor in my professional and personal development throughout the rest of my life.

I am grateful to my sponsors for their generous support during the course of my PhD (with supported work inside parentheses): National Science Foundation Career Award (for Chemical Mechanical Polishing), ICES-Dowd Fellowship (for Artificial Hip Joints) and Westinghouse Electric Company (for Mechanical Seals). I would like to thank the committee members: Prof.'s Robert Wood, Kurt Beschorner, Shi-chune Yao and Maarten deBoer for their valuable feedback on my thesis. I am thankful to the faculty members of the Mechanical Engineering department who enabled me to embark on the difficult path to a PhD. I would especially thank Prof. Yoed Rabin for his guidance in the subjects of Fluid Mechanics and Heat Transfer. I would also like to thank Prof.'s Jack Beuth and Phil Leduc for helping

me understand the nuances of solid mechanics.

I would like to thank all the present and past members of the PFTL who helped me at several stages of my research. Thanks to Dr. Jonatan Sierra-Suarez for all his help in the CMP project. Thanks to Patrick Dougherty for his support and guidance in the project for Artificial Hip Joints. I am also thankful to Dr. John Shelton for his invaluable contribution in the project for Mechanical Seals. Many thanks to the undergraduate researchers from the PFTL, especially Peter Chiappa and Graham Sides, who assisted me at several stages of my research. I would like to express my gratitude to the members of the PFTL for their thorough discussions during the group meetings and detailed review of presentations that helped me throughout the course of my PhD.

I would like to thank all my friends and family for bearing with me through long days and late nights for the past five years. Thank you Akanksha for keeping me sane through all the challenges of the PhD. Thanks to my sister Varsha, for all her love and kindness. Finally, I would like to thank my parents for their unconditional support throughout my life. Without their immense sacrifices, it would never have been possible for a middle class boy from an unremarkable section of central India to earn the highest degree from one of the best research institutions in the world.

Contents

Abstract	iii
Acknowledgements	vii
I Background and Development of Modeling Approach	1
1 Introduction	3
1.1 Regimes of Lubrication	4
1.1.1 Boundary lubrication	5
1.1.2 Hydrodynamic lubrication	5
1.1.3 Elasto-hydrodynamic lubrication	7
1.1.4 Mixed lubrication	7
2 Historical Review	11
2.1 Introduction to Tribological Modeling	11
2.2 Lubrication Regimes	12
2.3 Mixed Lubricated Interfaces	14
2.4 Simple (Hertzian) Sliding Contacts	19

2.4.1	Line Contact	19
2.4.2	Point Contact	20
2.5	Industrial Sliding Contacts	20
2.5.1	Artificial Joints	21
2.5.2	Internal Combustion Engine	22
2.5.3	Chemical Mechanical Polishing	24
2.5.4	The Particle Augmented Mixed Lubrication Approach	25
2.6	Conclusion	26
3	The PAML+ Modeling Approach	29
3.1	Physics behind the tribology	30
3.2	Model Development	32
3.2.1	Solid mechanics	32
3.2.2	Fluid mechanics	33
3.2.3	Particle dynamics	33
3.2.4	Wear	34
3.3	The PAML+ Modeling Approach	35
3.4	Applications	42
3.5	The Model's Name: PAML+ instead of PAML-lite	45
II	Applications of the Modeling Approach	47
4	Applications: A Textured Pin-on-disk Tribosystem Model	49
	Dougherty, P.S.M., Srivastava, G., Onler, R., Ozdoganlar, O.B., & Higgs, C. F., "Lubrication Enhancement for UHMWPE Sliding Contacts through Surface	

Texturing”, *accepted for publication in Tribology Transactions*(available online)

Currently under expansion

4.1	Introduction	49
4.2	Modeling Scheme	52
4.2.1	Hydrodynamic (lubricant) modeling	53
4.2.2	Pin-disk contact	54
4.2.3	Equilibrium Orientation	56
4.2.4	Friction	57
4.2.5	Wear	57
4.3	Experiments	58
4.3.1	Experimental setup	58
4.3.2	Surface texturing	59
4.4	Results	60
4.5	Load Carrying Capacity	61
4.5.1	Parametric Results	62
4.5.2	Model Limitations	65
4.6	Conclusion	66

5 Applications: Chemical Mechanical Polishing Model 69

Srivastava, G. & Higgs, C. F., “A Full Wafer Scale PAML Modeling Approach to Predicting CMP”, *accepted in Tribology Letters*(DOI : 10.1007/s11249 – 015 – 0553 – y)

5.1	Introduction	69
5.2	Modeling Scheme	71
5.2.1	Hydrodynamic (slurry) modeling	72
5.2.2	Wafer-Pad Contact	74

5.2.3	Equilibrium Orientation	76
5.2.4	Wear	77
5.3	Results	80
5.3.1	Fluid Pressure	82
5.3.2	Polishing Load	82
5.3.3	Particle Size and Concentration	84
5.3.4	Parametric Studies	87
5.3.5	Model Limitations	91
5.4	Conclusion	93
6	Applications: Artificial Hip Joints Model	95
	Srivastava, G. & Higgs, C. F., “Smart Artificial Hip Surfaces to Reduce Debris Contamination of Synovial Fluid”, <i>in preparation for Journal of Arthroplasty</i> Srivastava, G. & Higgs, C. F., “A Virtual 3D Multiphysics Tribological Model for Artificial Hip-Joints of Varying Surface”, <i>Orthopedic Research Society Annual Meeting Proceedings</i> , 2014	
6.1	Introduction	95
6.2	Modeling	97
6.2.1	Synovial Fluid	98
6.2.2	Acetabular Cup - Femoral Head Contact	101
6.2.3	Equilibrium Orientation	102
6.2.4	Debris Generation	104
6.3	Results and Discussion	106
6.3.1	Hip Motion and Loading	106
6.3.2	Lubrication fundamentals	115

<i>CONTENTS</i>	xiii
-----------------	------

6.3.3	Equilibrium orientation	116
6.3.4	Wear	117
6.3.5	Parametric studies	119
6.3.6	Model Limitations	128
6.4	Conclusion	130

7 Applications: Mechanical Seals Model	131
---	------------

Srivastava, G., Chiappa, P., Shelton, J. T., & Higgs, C. F., “A Fluid-Structure Interaction Model for Heat Transfer Analysis of Multiphase Flows in Tapered Non-Contacting Face Seals”, *Best Student Presentation awardee at STLE Annual Meeting 2015*

7.1	Introduction	131
7.2	Modeling Scheme	134
7.2.1	Fluid (hydrodynamic) modeling	136
7.2.2	Solid Deformation	138
7.2.3	Coupling	143
7.2.4	Dynamic Balancing	144
7.3	Results	146
7.3.1	Solution Procedure	146
7.3.2	Numerical Accuracy	148
7.3.3	Experimental Validation	149
7.3.4	Parametric Studies	151
7.3.5	Model Limitations	154
7.4	Conclusion	154

III Discussion	165
8 Conclusion	167
9 Impact and Future Work	171
9.1 Impact	171
9.2 Future Work	174
9.2.1 A Note of Humility from the Author to the Next Generation	174
IV Supporting Material	177
Appendices	179
A Industrial Scale Chemical Mechanical Polishing	181
Srivastava, G., & Higgs, C. F., “An Industrial-Scale, Multi-wafer CMP Simulation using the PAML Modeling Approach”, <i>accepted for publication in ECS Journal of Solid State Science and Technology</i> (available online)	
A.1 Abstract	181
A.2 Introduction	182
A.3 Modeling Scheme	184
A.3.1 Fluid Modeling	185
A.3.2 Wafer-Pad Contact	190
A.3.3 Equilibrium Orientation	192
A.3.4 Wear	193
A.4 Results	193
A.4.1 Shear Rates	193

CONTENTS

xv

A.4.2	Contact Stress	196
A.4.3	Fluid Pressure	196
A.4.4	Material Removal	197
A.4.5	Parametric Study: Platen Speed	198
A.5	Conclusions	199

B Thermal Effects in Chemical Mechanical Polishing 205

 Srivastava, G., & Higgs, C. F., “The Thermal Effects of CMP as a Particle Augmented Mixed Lubrication Tribosystem”, *MRS Online Proceedings Library, Volume 1560, 2013*

B.1	Abstract	205
B.2	Introduction	206
B.3	Modeling Scheme	207
B.3.1	Equilibrium orientation	207
B.3.2	Wear calculation	208
B.3.3	Temperature calculation	208
B.4	Results	210
B.4.1	Hydrodynamic pressure	210
B.4.2	Contact stress	211
B.4.3	Temperature map	211
B.4.4	Parametric study: Slurry viscosity	213
B.5	Conclusion	213

C Titanium Polishing in the Antek Stretch Polisher 215

C.1	Introduction	215
C.2	Literature Review	216

C.3	Sample Preparation	217
C.4	Handling	217
C.5	Recipe Recommendation	219
C.6	Modeling	220

List of Figures

1.1	The Stribeck curve: represents various lubrication regimes during the operation of a lubricated device	5
1.2	Stages in rough surface effects as lubricant film thickness reduces (from Spikes [1])	9
2.1	The Stribeck Curve, showing the variation in coefficient of friction as a function of the Sommerfeld number $S = \eta v/p$	13
2.2	Different categories of tribological models geared towards simulating multi-regime behavior	27
3.1	Schematic of a ball bearing (ref:www.spb-usa.com)	36
3.2	The degrees of freedom in a tribosystem. These are quantities that change by a small amount to allow the system to achieve load equilibrium	39
3.3	Applications studied through the PAML+ approach in this work .	44
4.1	Film thickness is assumed to be the mean separation between the pin and the disk	54

4.2	Different velocities in the system	55
4.3	Different pin geometries used in the simulations	56
4.4	Bruker UMT-3 tribometer used for the experiments	59
4.5	Experimental measurements of friction with increasing speed for several disk samples. All textures perform better than an untextured disk, with an intermediate texture size (and neither extreme) resulting in optimum performance.	64
4.6	Model predictions of friction with increasing speed for several disk samples. Similar to experiments, here both textures performed better than the untextured sample. Also, the lower texture dimension had a better frictional performance.	65
4.7	Model predictions of cumulative wear for several disk samples. An intermediate texture size ($200\mu m$) results in lowest amount of wear.	66
4.8	Contact stresses in a contact between a flat pin and a textured disk, for several Sommerfeld numbers. As the Sommerfeld number increases, the system moves from dry, or full contact, through different stages of mixed lubrication (fig. 1.2), to hydrodynamic or full film regime	68
5.1	Superposition of individual variables to calculate the film thickness	74
5.2	Different velocities in the system	75
5.3	Root finding algorithm	77
5.4	Flowchart of the modeling process	81
5.5	Dynamic fluid pressure profile for a well conditioned pad	83
5.6	Effect of polishing load on the material removal rate	84

5.7	Material removal rate with varying abrasive concentration in the slurry, plotted for various mean abrasive diameters. <i>Inset</i> : Data presented by Biemann	86
5.8	Material removal rate as a function of average particle size	87
5.9	Effect of newtonian slurry viscosity on the material removal rate .	89
5.10	Average fluid pressure as a function of viscosity (locally scaled Z axis)	90
5.11	Average fluid pressure as a function of viscosity (universally scaled Z axis)	91
5.12	Effect of particle size distribution on the material removal rate, for a mean particle size of 150 nm	92
6.1	Flowchart of the modeling process	99
6.2	Root finding algorithm	103
6.3	Three motions of the hip joint	107
6.4	Measured variation of flexion-extension angle α , abduction-adduction angle β , internal-external rotation angle γ and load L with time t	108
6.5	Data obtained from cite [1] after digitization	109
6.6	Curve-fitted, digitized data	110
6.7	Angular velocities obtained after differentiating the displacement curves	110
6.8	The two sets of coordinate axes: motion, and anatomical	112
6.9	Velocities along the anatomical coordinate axes, obtained after transforming the velocities along the motion axes	112

6.10	Forces along the anatomical coordinate axes, obtained after taking the components of the applied transient load along the anatomical axes	113
6.11	Velocities along the tribological coordinate axes, obtained after transforming the velocities along the tribological axes	113
6.12	Forces along the tribological coordinate axes, obtained after transforming the anatomical forces along the tribological axes	114
6.13	Summary of the motion and loading of the hip joint. Notice the three sets of coordinate axes: along the motion (flexion-extension, abduction-adduction, internal-external rotation), along the human anatomical axes (medial-lateral, superior-inferior, anterior-posterior), and along the tribological axes (X',Y',Z')	114
6.14	Material removal rate with different lubrication regimes	115
6.15	Sample output profiles from the model	117
6.16	Variation of volumetric wear with the size of the femoral head	118
6.17	Variation of wear rate with the size of the femoral head	120
6.18	Parameters required to define the surface texture	121
6.19	Variation in texture parameters	122
6.20	Instantaneous material removal, deposition over time	123
6.21	Effect of surface texture radius and maximum texture depth	124
6.22	Effect of separation between the textures (texture pitch)	126
7.1	The assembly for the No.1 seal in a reactor coolant pump. The coolant flows from a high pressure region to a low pressure region, between the two face plates	134

- 7.2 A schematic of the system being solved. The fluid flows from a high pressure region at R_o to a low pressure region at R_i through the gap between the two face plates. The fluid causes thermo-mechanical deformation in the surrounding face plates that have double- tapered geometry with minor and major taper angles as α_1 and α_2 respectively. The pressure within the seal gap is balanced by the closing load at the back of the seal assembly where the high pressure and low pressure regions are separated through the double-delta channel seal at the radial location of R_b 135
- 7.3 Proper sign convention for (a) Nodal displacements and slopes, (b) Transverse shear and bending moment, according to the theory of plates, and (c) Nodal forces and moments, according to finite element method; figures from [2] 139
- 7.4 Thermal boundary conditions for the face plates. The right edge is at equilibrium with the high pressure fluid at low temperature. The fluid goes through the seal gap, experiences high shear in the gap and with high viscous heat generation, comes out at higher temperature. The left edge of the plate is at equilibrium with this heated fluid. The top edge interacts with the fluid being heated and experiences a heat exchange with the fluid in the form of distributed flux. The bottom edge is assumed to be insulated 143
- 7.5 The fluid and the solid exist in a thermal equilibrium at the interface. The fluid and solid temperatures are equal at the boundary. Since there is no heat source or sink at the boundary, energy leaving the fluid should also be equal to the energy entering the solid 145

7.6	The flowchart for the EHL model. Note the inner “EHL loop” that ensures consistency between the fluid pressure and face plate mechanical deformation	156
7.7	The flowchart for the TEHL model. Even though the inner TEHL loop is shown here as a simple three step process, it is collection of several complex, coupled steps. See fig. 7.8 for the detailed TEHL loop	157
7.8	The TEHL loop that ensures consistency between the fluid pressure, the fluid temperature, solid temperature, and the face plate thermo-mechanical deformations	158
7.9	Leak rate as a function of grid size for low and high pressure gradients with inlet pressures of (a) 200 PSI, and (b) 2000 PSI, respectively. <i>Inset: Zoomed-in data</i>	158
7.10	Minimum film thickness as a function of grid size for low and high pressure gradients with inlet pressures of (a) 200 PSI, and (b) 2000 PSI, respectively. <i>Inset: Zoomed-in data</i>	159
7.11	Pressure and temperature along the mean film thickness as predicted by two models	159
7.12	Temperature distribution plotted over the fluid film geometry as predicted by two models	160
7.13	Leak rate as a function of inlet pressure (at OD) compared against other models and field data from Galenne and Pierre-Danos $\dot{V}_L$, measured at St. Albans power plant	160
7.14	Leak rate as a function of shaft speed for several inlet pressures. Outlet pressure fixed at 50 PSI	161

7.15	Temperature distribution within the fluid film for different shaft speeds and inlet pressures. Increase in viscous heat generation can be clearly seen as pressure gradients and speed increase	162
7.16	Leak rate as a function of shaft rotation speed for two different inlet pressures. Outlet pressure fixed at 50 PSI.	163
7.17	The variation in minor taper angle while keeping the major taper angle constant	163
7.18	Leak rate as a function of inlet pressure for different values of minor taper angles (in μrad). For higher pressure gradients TEHL model demonstrates near linear behavior with pressure, similar to fig. 7.13. Major taper: $600 \mu\text{rad}$, outlet pressure: 50 PSI	164
A.1	A schematic showing the arrangements of the wafer carrier over the pad. Also shown is the arrangement of six wafers within the wafer carrier.	186
A.2	Superposition of individual variables to calculate the film thickness	188
A.3	Velocities in the wafer carrier coordinate system (only 1 of 6 wafers shown). Radial ($v_{r(w)}$) and tangential ($v_{\theta(w)}$) velocities of any point on the wafer (having coordinates (r, θ) with the center of the wafer carrier as the origin), is the vector sum of the wafer rotation ($r_w \Omega_w$), and the wafer carrier rotation ($r \Omega_c$)	190
A.4	A sample surface topography of a section of the pad. The colours represent contact stress during a typical wafer-pad contact situation (see Sec. A.4.2) for more details	192

A.5	Fluid shear rate along the radial and tangential directions, at time step=0. This represents the complexity in the motion of the fluid within the interface, due to a combination of three rotations: of the pad, of the wafer carrier and of the individual wafers	195
A.6	Contact stress experienced by the asperities of the pad. At every time step, the contact stress and the fluid pressure, together, balance the applied polishing load.	196
A.7	Fluid pressure within the wafer-pad interface. (a), (b) show orthogonal views, and (c), (d) show contours of the pressure profile. The carrier is holding six wafers, as shown in (e)	201
A.8	Thickness of the Cu layer deposited on each of the wafers. Lower thickness reflects higher material removal. The positions of wafers changes with time due to the rotation of the wafer carrier. The position of each point on the surface of the wafer changes with respect to the corresponding wafer's center as well, due to the rotation of the wafer itself.	202
A.9	Variation of material removal rate with applied polishing load. Linear behavior is observed, that matches well with Preston's equation [3]: which relates pressure (P), sliding velocity (v) with wear volume (ΔV), as: $\Delta V = kPV$	203
A.10	Variation of material removal rate with the speed of rotation of the wafer carrier, for several platen speeds.	203
B.1	Dependence of interfacial fluid pressure on shear-rate	210

B.2	(a) Variation in contact stress in the pad, (b) Corresponding flash temperatures	211
B.3	Temperature maps (a) Pad temperatures (b) Wafer temperatures (c) Interfacial fluid film temperatures	212
B.4	Variation in temperature rise and MRR with viscosity	214
C.1	Comparison in edge quality of wafers obtained through abrasive water-jet cutting and wire EDM	218
C.2	Surface profile of a polished surface extracted from Zygo NuView 6300 optical profilometer	220
C.3	Predictions of material removal using PAML+ for conventional polisher	221
C.4	Contact stress between a sinusoidal surface and another flat surface	221
C.5	Antek stretch polisher: major components and motions	222
C.6	PAML+ for Antek stretch polisher: sample output	223
C.7	Comparison of material removal rates between a conventional rotary polisher and the Antek stretch polisher	223

List of Tables

4.1	Texture dimensions	60
4.2	Model Parameters	61
5.1	Model Parameters	80
7.1	Model Parameters	146
A.1	Model Parameters	194

Nomenclature

α	Orientation of the wafer with X-axis
α_1	Minor taper angle in the face plate
α_2	Major taper angle in the face plate
β	Orientation of the wafer with Y-axis
δ_0	Z-separation between the wafer center and mean plane of the pad
η	Slurry viscosity
λ	Dimensionless coefficient
ν	Poisson's ratio
ν_{pad}	Poisson's ratio of the foundation (pad)
Ω_c	Angular velocity of the wafer carrier
Ω_d	Angular velocity of the disk
Ω_p	Angular velocity of the pad
Ω_w	Angular velocity of the wafer

Ω_{pin}	Angular velocity of the pin
ϕ	Density ratio ($= \rho / \rho_c$)
Φ_s	Shear flow factor
$\Phi_{r/\theta}$	Radial / Tangential flow factor
ρ_f	Density of the fluid
$\sigma(x,y)$	Contact stress at position (x,y)
σ_d	Standard deviation in the diameter of abrasives
τ	Initial height of the foundation
θ	Tangential coordinate measured from X-axis of the face plate
θ	Tangential coordinate measured from X-axis of the wafer
θ_{wc}	Tangential coordinate of a wafer center, changes with time due to the rotation of the wafer carrier
Δ	Combined indentation of the particle into the pad and wafer
Δ_p	Indentation of the abrasive into the pad surface
Δ_w	Indentation of the abrasive into the wafer surface
a_i	Radial coordinate of the i-th node
a_w	Width of contact between an abrasive and the wafer surface
C_f	Specific heat capacity of the fluid

d	Diameter of an abrasive particle
d_{avg-a}	Average diameter of active particle
d_{avg}	Mean diameter of abrasives
E	Elastic modulus of the face plate
E_{pad}	Elastic modulus of the foundation (pad)
F	Force on the abrasive while indenting on the wafer
F_z	Net force on the wafer, along the Z axis
$F_{closing}$	Gap closing force
$F_{opening}$	Gap opening force
g	Switch function
h	Fluid film thickness
h_0	Axial translation of the stator
H_w	Hardness of the wafer
k_f	Thermal conductivity of the fluid
k_s	Thermal conductivity of the solid
M_r^K	Radial moment
M_x	Net moment on the wafer, along the X axis
M_y	Net moment on the wafer, along the Y axis

N	Number of abrasive particles
p	Hydrodynamic fluid pressure
P_{high}	Pressure at the outer radius, seal upstream pressure
P_{low}	Pressure at the inner radius, seal downstream pressure
Q_r^K	Transverse shear force
r	Radial coordinate with shaft center as the origin
r	Radial coordinate with wafer center as the origin
R_b	Balancing radius, radial location of the double-delta channel seal
R_c	Radius of the wafer carrier
R_i	Inner radius of the annular face-plate
R_o	Outer radius of the annular face-plate
R_t	Radial location where the minor and major tapers meet
r_{pd}	Separation between the axes of rotation of pin and disk
r_{wc}	Separation between the axes of rotation of a wafer and the wafer carrier
r_{wp}	Separation between the axes of rotation of wafer and pad
t_p	Plate thickness
$u(x,y)$	Z-deflection at position (x,y)
u_r/θ	Radial / Tangential velocity of the fluid

$v_{\theta(p)}$	Velocity of the pad in the tangential direction
$v_{\theta(w)}$	Velocity of the wafer in the tangential direction
$v_{r(p)}$	Velocity of the pad in the radial direction
$v_{r(w)}$	Velocity of the wafer in the radial direction
v_{rel}	Relative velocity between an abrasive and wafer surface
Vol_{avg}	Average material removed by an active particle
w^K	Nodal deflection

Part I

Background and Development of Modeling Approach

Chapter 1

Introduction

Tribology or the study of friction, lubrication and wear is crucial to our modern lifestyle. Our life now revolves around machinery that uses rolling and sliding contacts. In some cases, these machines benefit from friction, in certain others, they suffer degradation and loss of functionality. Some examples of productive friction and wear are walking, writing with a pencil, brakes, clutches, machining and shaving. Examples of counter productive friction occur in engines, gears, cams, bearings and seals.

High friction and wear cause energy loss and deterioration of interacting surfaces. Estimated losses to industries due to “wear and tear” are approximately 12% of the GDP. For the UK, 2% of the GDP is about £28B. For the US, it is a staggering \$300B. Not just that, approximately a third of the world’s energy resources are lost in friction in one form or the other. Lubrication, using solid or fluid lubricants is the primary mechanism to reduce friction and wear. Solid lubricant is any material that results in a thin solid film on a surface to provide protection from damage during

relative movement. Solid lubricants are used in applications where low speed sliding contact occurs, for example a bearing operating at high loads and/or low speeds, or a lubricated bearing requiring frequent start-stop operations. A thin fluid film on the order of surface roughness of the surfaces results in lower friction and wear. A thick fluid film between two solid surfaces prevents solid-solid contact and can provide very low friction and negligible wear.

1.1 Regimes of Lubrication

The regime of lubrication where a fluid film is maintained between two surface through an external pumping agent, is called hydrostatic lubrication. This regime is also characterized by little or no relative motion between the solid components.

All other fluid-mediated sliding contacts which persist in the absence of an external pumping agent can be represented through a Stribeck curve [Stribeck (1902)], shown in Fig. (1.1). The Stribeck curve represents the coefficient of friction between the two components as a function of the lubricant viscosity, relative velocity and the carried load. It can be observed that the curve has a non-monotonic behavior with a minimum, which indicates that there are more than one mechanisms which cause the friction. Explanation for these different lubrication regimes have been proposed by several authors in the past. A brief description of the major lubrication regimes is presented here.

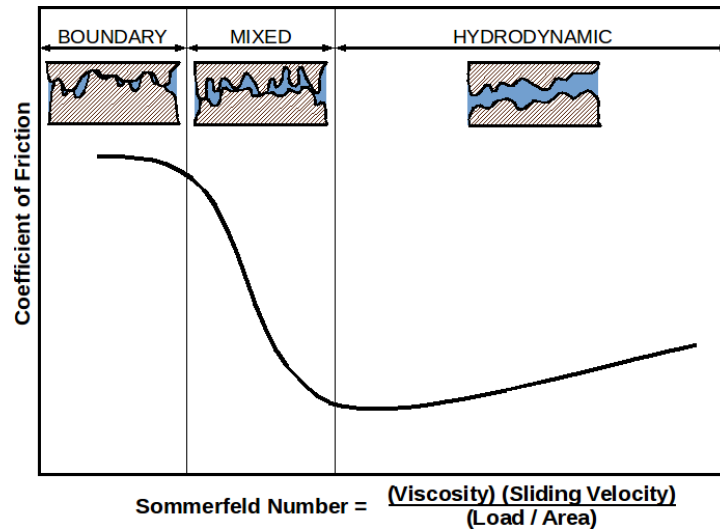


Figure 1.1: The Stribeck curve: represents various lubrication regimes during the operation of a lubricated device

1.1.1 Boundary lubrication

At high loads, and/or low velocities, and/or low viscosities, the interface appears to be in the “starved” condition. In this regime, the solid surfaces are so close together that the interactions between the asperities and the molecular interactions between the solids and lubricant films dominate the contact. Under the influence of such interactions, the coefficient of friction rises sharply and approaches high values that are virtually independent of load, velocity and lubricant viscosity.

1.1.2 Hydrodynamic lubrication

At the other extreme, under lower loads and/or, high relative velocities and/or, high viscosity, the interface is in the “flooded” condition. This regime is called the hydrodynamic (HD) lubrication, or sometimes the full-film lubrication. When a fluid is entrained into a converging gap due to the relatively moving surfaces, it

is compressed between the solid boundaries and develops sufficient pressure to support the load. This is the mechanism of hydrodynamic lubrication and is critical to the operation of journal and thrust bearings.

Fluid films can also be generated by motion normal to the solid surfaces. This mode of lubrication is called “squeeze”, and can be fixed or variable in magnitude referring to steady state or transient lubrication, respectively. This mechanism is driven by the fact that the lubricant cannot be instantaneously squeezed out of the interface due to its viscosity. This resistance to extrusion from the fluid governs the buildup of water films under the tires of automobiles and airplanes on wet tarmac, commonly known as hydroplaning, even in the cases of virtually no relative motion at the point of contact.

The hydrodynamic lubrication regime is generally considered to be the favorable lubrication regime as the film thicknesses are much larger than the dimensions of the asperities. This means that there is almost no solid-solid contact and the friction coefficients can be very low (as low as 0.001). However, the viscous drag from the lubricant does increase the friction with increase in the relative velocity. No solid-solid contact also means that there is low possibility of abrasive, adhesive or any other contact driven wear. Unfortunately, the need for high velocities or viscosity limit the application of hydrodynamic lubrication regime to highly specialized industrial applications that have the capacity to expend the power required to produce such high shaft velocities or spin such high viscosity fluids.

1.1.3 Elasto-hydrodynamic lubrication

Elasto-hydrodynamic lubrication (EHL) is a subset of hydrodynamic lubrication where the elastic deformation of the solid surfaces plays an important role in the lubrication process. The film thicknesses are much smaller than in conventional hydrodynamic lubrication, and are still capable of supporting the entire load. EHL is most commonly induced in systems where heavy loads act on relatively smaller contact areas, such as point or line contacts of rolling element bearings and gear teeth. It can also set up in cases where the solid surfaces have relatively low elastic moduli or high conformity, such as in the cases of lip seals, journal bearings with soft liners and head-disk interface in magnetic storage drives. Under heavy loads, high fluid pressure can lead to both changes in the viscosity of the lubricant and elastic deformation of the surfaces. These two effects in combination lead to changes in the geometry of the bounding solid bodies, thus making the analysis of such interfaces more complex. In general, computation modeling of EHL deals with simultaneous resolution of fluid pressure and elastic deformation of the solids, while accounting for the changes in the viscosity of the fluid with the fluid pressure.

1.1.4 Mixed lubrication

The evolution of the lubrication mechanism from boundary to hydrodynamic lubrication during cases such as a bearing startup passes through the zone known as mixed lubrication. Here, both the mechanisms play significant roles: there might be solid-solid contact, but a portion of the applied load remains supported by the fluid film. With decrease in the load and/or, increase in the relative velocity and/or, increase in the fluid viscosity, the load being carried by the fluid film increases,

reducing the coefficient of friction as shown in Fig (1), until the entire load is supported by the fluid, thus completing the transition to hydrodynamic lubrication. The mixed lubrication regime offers a trade-off between the high frictional losses of boundary lubrication, and high power costs to generate full film lubrication. Due to this tribologically efficient nature of the “mixed” contact, a wide variety of natural and industrial applications operate in the mixed lubrication regime. Some common examples are listed below:

- **Lapping, Honing and Polishing:** The applied load is supported by both the polishing slurry and the solid-solid contact between the polishing pad and the workpiece. Abrasives present in the slurry are the wearing agents that result in high precision wear action.
- **Synovial joints:** The load transferred across the joints i.e. the entire body weight in the case of hip or knee joints, for example, is shared by cartilage-coated bone-bone contact and the synovial fluid. In the artificial joints this contact is replaced by the metal-metal or metal-polymer contact, while part of the load is still supported by the synovial fluid.
- **Degradation of teeth through food:** While chewing the food, the load is supported by the contact between the teeth and the squeeze resistance of saliva or other liquids if present. Presence of abrasive particles leads to corrosive wear of tooth enamel.
- **Lubrication of piston rings in an internal combustion engine:** The load generated by thermo-elastic expansion of the piston rings is supported by the solid-solid contact between the cylinder bore and the rings, and partially by

the “engine oil”. Presence of solid contaminants or unburnt carbon particles leads to the wear of piston rings, that causes loss of compression and thus loss of power in the engine.

Stages of mixed lubrication

Before we go into the details of mixed lubrication modeling, it is important to study the different stages mixed lubrication acts in. When the interface transitions from a separated full-film lubrication regime to a boundary lubrication regimes, it passes through five stages. These are shown, schematically in Fig. 1.2. At the beginning,

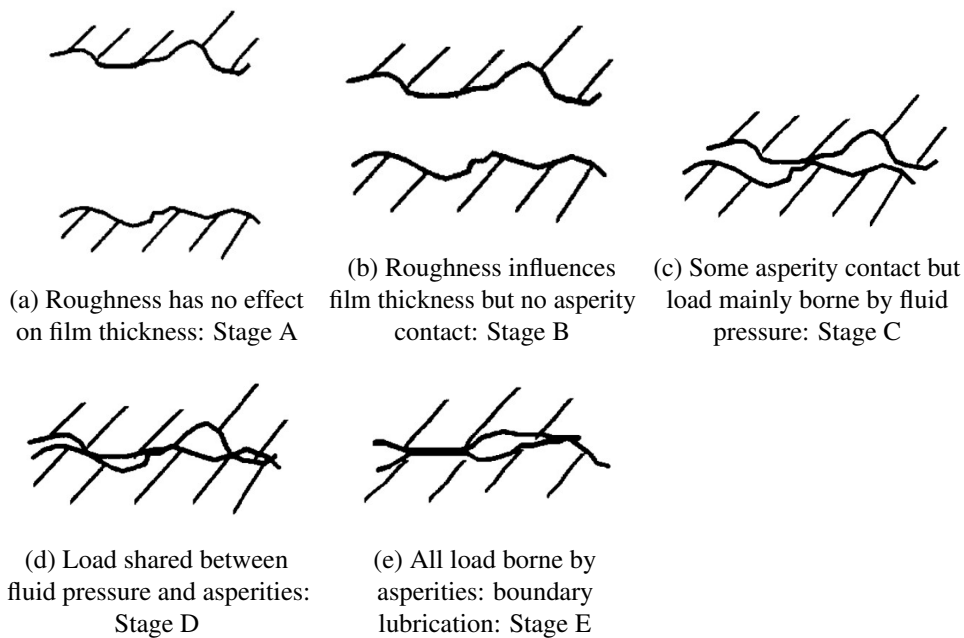


Figure 1.2: Stages in rough surface effects as lubricant film thickness reduces (from Spikes [1])

the film thickness will be much larger than the roughness of either of the surfaces. As a result, the roughness will have almost no effect on the fluid flow, friction or the

load carrying capacity of the interface (Fig. 1.2a). Friction would be low as the only contributor is the viscous shearing of the fluid. As the load increases or interface slows down, thus reducing the Sommerfeld number, the roughness starts influencing the flow, and affects the fluid flow and the load carrying capacity. However, inspite of the roughness affecting the fluid flow, there is still negligible contact between the two surfaces (Fig. 1.2b). Friction would remain relatively low even though viscous shearing has slightly increased. When Sommerfeld number reduces further, there are a few points of contact between the two surfaces, and the fluid is getting strongly influenced by the roughness of the surfaces (Fig. 1.2c). This partial contact would also affect the performance and friction would start increasing with occasional asperity collisions and adhesion. However, the load is still being carried almost entirely by the lubricant. In the next stage, the load starts getting shared similarly by both the fluid and the solid-solid contact (Fig. 1.2d). The mean separation between the two surfaces is now getting influenced by the roughness of the two surfaces and the load carrying capacity of the fluid. Also, the friction starts rising as the “boundary” component of the contact starts increasing in magnitude, while there is still influence of viscous shearing. Lastly, at very low Sommerfeld numbers, the fluid film becomes so thin that there is negligible fluid pressure and the entire load is being carried by the solid solid contact and the resultant friction is also much higher (Fig. 1.2e).

Chapter 2

Historical Review

2.1 Introduction to Tribological Modeling

Friction and wear modeling is important for design engineers. Dry and lubricated contacts are omnipresent across all devices and govern the running quality of machines. There are two aspects to this tribological modeling: friction, and wear.

Friction: Historical records from the sixteenth century have revealed that famous engineer and artist Leonardo da Vinci proposed the concept of a coefficient of friction that related the normal force and sliding resistance, or “friction” force. Guillame Amontons, a French physicist later in 1699 established the significance of the coefficient of friction which was found to be independent of the apparent area of contact. Another French physicist Charles-Augustin de Coulomb discovered that this coefficient of friction is different in stationary contacts, and sliding contacts, and thus, called them static and kinetic coefficients of friction respectively. It was also observed that the kinetic friction was independent of velocity. Bowden and

Tabor, for the first time, in 1950 elucidated the mechanisms for reducing friction and wear through surface interactions in the form of soft coatings and molecular adherence.

Wear: Wear has always been considered a very complex process and general theories are very rare. The most common modeling approach for wear has been through a large swath of empirical equations. Archard's wear law [4] introduced in 1953 related the applied load F , relative sliding distance d , indentation hardness H with the worn volume V , through a dimensionless wear coefficient k : $V = kFd/H$.

2.2 Lubrication Regimes

Several distinct regimes are employed to describe the fundamental principles and tribological behavior of interfaces. One can imagine that a tribosystem consists of two surfaces in relative sliding motion with the intervening media between being a lubricant, wear debris or particles, and/or just empty air. Assuming the top surface is imparting a load to the interface, the frictional regimes that exists primarily differ in the way in which the load carrying mechanism occurs. These regimes range from a *dry sliding* regime, to completely separated contact in the form of *full-film lubrication*, with an intermediate regime involving partial contact in the form of *mixed* lubrication. Also, when deformation of the surface impacts the fluid film lubrication, as in the case of roller bearings, or gear teeth, elasto-hydrodynamic lubrication (EHL) regime brings in distinctive characteristics. Figure 2.1 shows the Stribeck curve that is utilized to represent the frictional behavior of a tribological interface, as a function of several operating parameters.

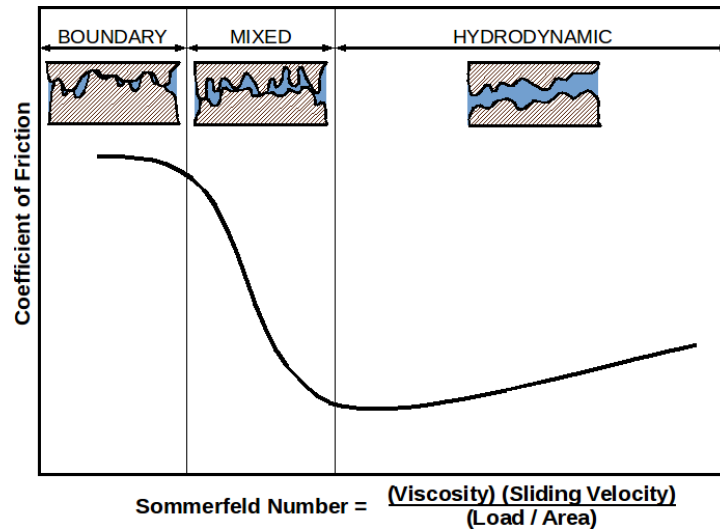


Figure 2.1: The Stribeck Curve, showing the variation in coefficient of friction as a function of the Sommerfeld number $S = \eta v / p$

A complete tribological model should seamlessly be able to traverse these distinct, but connected lubrication regimes. As seen in subsequent sections, very few authors have attempted to simulate multiple lubrication regimes through a single modeling framework. The primary hurdle in constructing a unified model is the physical complexity of the mixed lubrication regime. The extraordinary level of physical action in the interface during mixed lubrication makes its simulation an arduous task. *Thus, the development of unified approaches, however rare they are, has followed the development of frameworks capable of handling mixed lubrication lubrication regime.*

2.3 Mixed Lubricated Interfaces

The term “mixed friction” was first recognized in the literature around 1930s by Felz. It later evolved into “mixed or quasi-hydrodynamic lubrication” through Cameron’s landmark textbook in 1966 [5]. As mentioned in last chapter, mixed lubrication refers to a state of lubrication where the applied load on the interface is supported by both the fluid pressure, and the contact stress between the two solids. Even though mixed lubrication has been recognized for quite a while now, its current understanding remains rudimentary at best. Its progress depends heavily on breakthroughs in two areas: an integrated understanding of the boundary and hydrodynamic lubrication regimes, and sufficient knowledge of the stochastic nature of the rough surface interaction. With the introduction of Greenwood and Williamson’s seminal contact formulation [6], and inception of a multitude of elasto-hydrodynamic lubrication theories, the mid to late 1960s saw extraordinary growth in mixed lubrication studies.

Since then, a large number of mixed lubrication models have been presented focusing on both industrial and academic tribosystems. Contributions have been split in two different aspects of the mixed lubrication analysis. First is the full solution of fluid film thickness and pressure in the case of mixed contact. The other is towards the study of load sharing between hydrodynamic pressure and solid contact stress. This concept of “load sharing” or superposition of loads carried by the two mechanisms has gained popularity as it was relatively straightforward.

The earliest attempts at simulating mixed-EHL lubrication was for the stage B shown in fig. 1.2b, i.e., the stage in which the film thickness is larger than the rough-

ness, but is still being influenced by the asperities. One of the first studies was done by Michell in 1950, where he assumed sinusoidal asperities on a pivoted pad thrust bearing to calculate the load carrying capacity (LCC). Similar to a classic Stribeck curve, he predicted a minimum in bearing friction, and a slight drop in LCC, when the film thickness was comparable to the amplitude, or the height of the asperities. This was later extended by researchers to other forms of roughnesses.

All of these earlier studies were deterministic, by prescribing a known height distribution to a nominally smooth surface. The effect of statistically rough surface was first studied by Cheng [7,8] and Elrod [9] through their “average flow” model. Christensen proposed another approach to this, through his expectancy analysis [10, 11]. It was generally concluded that transverse, or the profile perpendicular to the sliding direction would enhance LCC, while longitudinal, or parallel to the sliding distance would decrease LCC. In all of the above, and follow on works, the effect of asperities was only considered on the hydrodynamic pressure. The possible LCC of direct asperity contact was not considered.

Through seminal experimental work by Tallian et al. [12] and Czichos [13], the role of asperity contact in lubrication was demonstrated as the film thickness reduced further to the scale of the asperities. These interactions were later modeled independently by Johnson [14] and Tallian [15]. Both authors developed load sharing mechanisms between the fluid pressure, and the asperity contacts between Gaussian surfaces. Johnson followed Greenwood and Williamson’s model [6, 16] for elastic contact between asperities whereas Tallian’s work also allowed the asperities to deform plastically. Both authors, however, neglected the effect of roughness on the fluid flow, contrary to the work by Elrod [9], Cheng [7,8] and Christensen [10, 11] mentioned earlier.

It did not take researchers much time to understand that the fluid pressure could influence the shape of the asperity, and, an asperity could affect the fluid pressure as well. It was a possibility for both rough surface hydrodynamic and elasto-hydrodynamic lubricated contacts, that the asperities start deforming under fluid pressure and effectively form tiny ‘micro-elastohydrodynamic’ (micro-EHD) contacts.

The natural approach forward was to solve the EHL problem with the rough surface profile as is done for a smooth surface, i.e., simultaneously solving the Reynolds equation, elasticity equation and load balance. However representing such rough surface computationally needed very high resolution meshes and would require enormous computing resources for the solution. Moreover, unlike a smooth solution where the gap remains constant over time, a rough simulation is inherently a transient simulation thus making the problem even more computationally expensive.

Almost all authors approximated the contact of two rough surfaces to a contact between a smooth surface and a surface with roughness equivalent of the two initial surfaces. Such rough-on-smooth contact, while in EHL, would lead to flattening of the asperities. The flattening effect was observed to be more pronounced in stationary contacts, than in moving contacts [17].

Since the first investigation by Chang et al. in the mid-90s there have been very few transient, rough-surface EHL modeling approaches [18–21]. Some of them would be discussed later in the section. The works discussed above, however, did not account for possibility of asperity contacts and thus the LCC of “boundary” films.

The natural progression beyond the above work was to combine the micro-EHD modeling with the load sharing concepts. So far, there have been very few such attempts. Earliest work is attributed to Patir and Cheng during their development of the average flow models. They used elastic asperity deformation in their statistical approach showing the difference in the film thicknesses and resulting LCC for isotropic, transverse and longitudinal roughness profiles. Similar approaches were followed by Majumdar and Hamrock [22] and Zhu and Cheng [23, 24] but are all considered limited in their application as the statistical models are not well suited for cases where the film thickness is comparable to the asperity heights. Later on, Chang [25] presented an innovative deterministic solution approach which simultaneously solves the Reynolds equation, the elastic deformation for the solids, and asperity contact interactions. This approach has been successful at predicting the occurrence of film collapse, and large scale pressure fluctuations in the vicinity of asperity contacts.

Significant advancements in computational power has fueled breakthroughs in thin-film EHL and mixed-lubrication research since mid-1990s. Improved optical interferometry has yielded experimental evidence of the importance of ultrathin film and boundary lubrication, and has provided researchers motivation to study these complex problems. Guangteng and Spikes [26], Luo et al., Kaneta and Nishikawa [27], Luo and Liu, and Krupka and Hartl [28] are considered the major contributors in conducting these experimental studies.

Modeling with Deterministic Surfaces. In parallel, deterministic modeling approaches for mixed lubrication have made significant progress. There have been

two distinct set of approaches being followed. The first uses separate models for lubrication and contact modes. The second is the unified equation approach that uses one single equation for both lubricated zones and asperity contacts in the interface. Chang [25, 29] presented the first separate models approach for line contact with three-dimensional roughness. It was soon followed by Jiang's work [30, 31] for point contacts operating in mixed lubrication with machined roughness. Later on, this separate models approach has been carried forward by Zhao et al. [?, 32, 33], Holmes et al. [34], Zhao and Sadeghi [35], and Popovici et al. [36], mainly for transient problems such as start-up and shut-down of machine components such as bearings. The first unified approach for point contacts with machined roughness was published by Zhu and Hu [23], and later by Hu and Zhu [37]. Holmes et al. [38, 39], using coupled differential deflection method presented another unified approach. Li and Kahraman [40, 41] employed asymmetric integrated control volume discretization for their unified approach towards mixed lubrication.

In recent years the research around mixed lubrication has been observed to bifurcate into two distinct sections. One section studies fundamental tribological problems, such as Hertzian point and line contacts under the mixed lubrication regime. The other section develops modeling solutions dedicated to applied, industrial tribological problems. Major contributions in either of these domains are going to be highlighted in the following sections of this chapter.

2.4 Simple (Hertzian) Sliding Contacts

Most of the research dedicated in pushing the limits of the current tribological modeling capabilities deals with simplified contacts to reduce the complications arising from complex operating conditions. The simplest of the tribosystems are the Hertzian line and point contacts. Since the understanding of the tribological mechanisms in both of these systems is quite mature, only the major milestones are highlighted in this section.

2.4.1 Line Contact

The earliest established works in deterministic characterization of mixed-lubrication in line contacts was presented by Chang [25,29]. He combined the concepts used in stochastic and deterministic modeling of micro-EHD contacts, to simulate transient line contact problems. He assumed the contact to be frictionless, elastic, isothermal interaction. Polycarpou and Soom [42] gave another semi-empirical model that accounted for partial contact between two sliding components in a lubricated line contact. They explicitly decomposed the friction into solid (asperity contacts) and fluid shear components. Building on Johnson's work [14], Gelinck and Schipper [43] gave a model capable of simulating deterministic rough line contacts. They combined the EHL regime with the rough contact in mixed-lubrication regime to construct a framework to simulate the frictional behavior represented in the Stribeck curve. Recently, Ren et al. [44] presented a 3D deterministic model for rough line contacts based on Hu and Zhu's approach [37] to simulate mixed, point contacts, combined with Chen et al.'s [45] DC-FFT approach to calculate solid deformation.

2.4.2 Point Contact

Jiang et al. [30] presented a deterministic approach that solved hydrodynamic pressure and asperity contact stress simultaneously. They used multi-grid scheme to solve Reynolds equation for fluid pressure and FFT procedure to calculate solid deformation and contact stress. Hu and Zhu [37] presented a full numerical solution to mixed lubrication in point contacts. Contrary to prior studies who used hypothetical, simplified topographies, Hu and Zhu implemented measured real 3D topography. Their approach was able to model the entire range of lubrication regimes, from boundary to full film hydrodynamic lubrication, for a range of rolling and sliding velocities. Wang et al. [46] presented another transient approach for modeling point contacts operating under mixed lubrication and calculated temperature rise, together with the fluid pressure and asperity contact stresses in the interface. Holmes et al. [34] presented a transient technique for modeling mixed lubrication in point contacts in gear teeth. They simulated transverse ground surfaces in elliptical contacts undergoing severe film thinning and high fraction of asperity contacts. More recently, Sojoudi and Khonsari [47] have presented a simple, semi-empirical model to predict friction in lubricated point contacts. They applied the load sharing concept to isolate the dry contact component and lubricated contact components. They used the model to predict the lift-off speed for sliding, rough, lubricated contacts.

2.5 Industrial Sliding Contacts

As mentioned in the previous sections, contrary to the research conducted in simpler contacts, real systems involve complex motion and loading conditions that vary with space and time. Hence the models developed to tackle industrial problems tend to be

very limited in their scope, and are generally only applicable to a very limited set of conditions. Since industrial tribo-systems are also much larger (relative to simpler line and point contacts), the industrial modeling frameworks also tend to have reduced order physical models when compared to the simpler contacts. For example, several authors have utilized high fidelity, high mesh density, finite element analysis (FEA) to study the solid deformation in the case of a point contact of rough surfaces. However, detailed FEA studies involving rough surface contact in chemical mechanical polishing are virtually non-existent. Similarly, some authors have also simulated the behavior of a multi-component lubricant made of immiscible fluids (water and oil, for example) in a line contact through multi-phase, turbulent, computational fluid dynamics (CFD). However similar high-fidelity studies involving complex CFD are absent from similar analysis for internal combustion engines. A few such modeling attempts for some important industrial applications that operate in the mixed lubrication regime are discussed in the sections below.

2.5.1 Artificial Joints

An artificial hip joint is essentially a spherical bearing where the two bearing surfaces are sliding against each other in the presence of a lubricant known as the synovial fluid. Extremely high loads, low velocity and relatively low lubricant viscosity mean that the artificial hip joint normally operates in the boundary or mixed lubrication regime. However, in the literature, there are only a few recent works on mixed lubrication modeling of artificial joints, most likely due to the complexity of modeling the mixed lubrication regime, as opposed to a purely singular phenomenon regime, such as boundary lubrication (solid-solid sliding contact) or full film, hydrodynamic lubrication. Jin [48] presented an empirical

model to offer theoretical explanation for the experimental observation of Smith et al. [49], who conducted measurements for ceramic-on-ceramic hip joint prosthesis. He used the Greenwood and Williamson's asperity contact model [6, 16] and Patir and Cheng's average flow model [7, 8] to calculate the load sharing between the fluid pressure and asperity contact stresses. Most relevant models are due to Wang who proposed both direct and indirect contact analyses [50–52]. In Wang et al. [53] a steady state mixed lubrication model of metal-on-polymer joint was investigated through the EHL modeling equations for the fluid pressure, and an inverse filter plus smooth function method (IFM) for contact mechanics. Wang later presented another transient model of mixed lubrication in metal-on-metal hip joints. EHL modeling was coupled with an indirect contact model, based on simplified Reynolds equation with Poiseuille terms removed. They simplified the analysis by assuming the surfaces to be smooth, but allowed a thin protein layer to form on the solid components, thus adding another level of complexity. They showed that metal-on-metal joints also operated, prevalently, in the mixed lubrication regime. They validated their approach by comparing their predictions of frictional torque on the bearing surfaces, against experimental measurements.

2.5.2 Internal Combustion Engine

The sliding contact between the piston rings and the cylinder bore is lubricated by the engine oil - fuel mixture. The piston rings are designed such that there is partial contact between the asperities of the ring and the cylinder bore, thus limiting the fluid leakage through the gap, while still providing lubrication while sliding. High pressure in the combustion chamber and high sliding velocity lead to significant wear and cause loss of performance in the engine. The tribology

of the interface, specially at the extreme conditions inside an IC engine are of significant interest to the automotive industry. Akalin and Newaz [54] simulated the first compression ring in a typical diesel engine. They presented an axi-symmetric, mixed lubrication model using average flow Reynolds equation, and asperity contact to simulate frictional performance of piston ring and cylinder liner. They concluded that the system operates in hydrodynamic lubrication regime for the most part of the stroke, but mixed lubrication occurs at the top and bottom dead centers due to high cylinder pressure, and low sliding speeds. Livanos and Kyrtatos [55] presented a friction model for a marine diesel engine piston assembly. It accounted for the combined effect of the friction at compression rings, oil control rings, piston skirt and gudgeon pin on the engine piston assembly. Priestner et al. [56] presented a model to study wear profiles of slider bearings to achieve better friction prediction. Their model accounted for fundamental characteristics of engine operation such as load, temperature, shaft speed and oil characteristics. They used Reynolds equation to simulate the fluid behavior and Greenwood and Tripp [16] to model asperity contacts. Ma et al. [57] presented a 1D mixed-EHL model to study friction and wear in cylinder liners and pistons. The model accounted for the effects of surface roughness, temperature, oil viscosity on wear and lubrication. They used empirical wear law to calculate material removal using the asperity contact stress. They deduced that the sliding friction achieves a minimum value at certain oil temperatures. Zhu et al. [24] presented another model for piston skirts operating in mixed lubrication. They accounted for the effects of surface roughness and waviness, piston skirt surface profiles, bulk elastic deformation and thermal distortion of both piston skirt and cylinder bore on piston motion, lubrication and friction. They used the model to simulate the piston trajectory, and studied the friction as a function of

crank angle under the engine running condition.

2.5.3 Chemical Mechanical Polishing

Chemical mechanical polishing (CMP) is the classic example of a mixed lubrication tribosystem. It is such a clear, well-researched, mixed lubrication problem that it is routinely discussed in Tribology courses. The applied polishing load is carried by the solid-solid contact between the polishing pad and the wafer and the hydrodynamic pressure in the polishing slurry. However together with the partial contact, abrasive particles cause material removal from the surface of the wafer which makes the overall tribology of the process extremely complex. Combined with the presence of chemical actions, CMP is generally considered an extremely difficult problem to model, and empirical models are the only reliable source of guidance for the industry. However, over the years few authors have attempted to model the mechanical action undergoing in the interface. Shan et al. [58] presented a seminal model that simulated the CMP process as a rough contact problem between a rigid, flat punch against an elastic half space, in the presence of an abrasive slurry. Through this simplified model they were able to explain the presence of a sub-ambient, or negative fluid pressure region under the wafer that presumably causes higher non-uniformity in material removal across the wafer. Seok et al. [59] then presented a multi-scale mixed lubrication model that coupled the solution of solid solid contact with the fluid pressure, and enforced the global force and moment balance. They also accounted for large deformations in the compliant pad by introducing a hyperelastic material in their asperity scale interactions, that were simulated through finite element analysis. They concluded that because of this highly compliant behavior of the pad at different roughness scales, non-uniformity in material removal would

be unavoidable with either concave, convex, or flat wafers. Higgs et al. [?] then presented a three-dimensional wafer-scale model explaining the negative pressure under the wafer. Their model also ensured global force and moment balance, and incorporated frictional interaction during relative sliding between the wafer and the pad. Even though they used a much simpler contact stress formulation, in the form of Winkler elastic foundation method, their results matched the higher accuracy methods employed by previous authors. Around the same time, Jin et al. [60] presented another three-dimensional, wafer scale model for CMP by coupling the fluid flow solution with the micro-scale asperity contact. Using the Winkler Elastic Foundation method, they also accounted for the bulk pad deformation due to solid solid contact and fluid pressure. They modified the fluid solution to account for the high compliance in the pad, thus constructing a “soft-EHL” framework.

All these models above, however, neglected, or heavily approximated the most important component of chemical mechanical polishing: wear. All the models above have also accounted for the roughness of the surface in a statistical manner. Lack of wear predictions, and absence of any deterministic information made the models less useful for the CMP industry directly where the biggest objective of CMP research is to improve the polishing efficiency.

2.5.4 The Particle Augmented Mixed Lubrication Approach

In 2009 Terrell and Higgs [61] presented a new multiphysics approach to modeling the CMP process. Instead of modeling the fluid flow with the Reynolds lubrication equation, utilized three-dimensional Navier Stokes equations to study the behavior of the fluid. Similar to several authors in the past, they used Winkler Elastic Foundation

method to account for partial contact between the pad and wafer asperities. They employed Lagrangian particle tracking to study the particle-particle and particle-surface interactions. With extensive information about individual particles, they were also able to simulate abrasive wear behavior to study the material removal process. However, these high fidelity sub-models came at very high computational costs and limited the domain that could be studied. Spatially, the solution was limited to a square of side of about $25\mu m$, and temporally to a few microseconds. Their framework was highly accurate, but due to the high computational costs, it was not directly relevant to the CMP industry. This meant that even though the model was intended for the “industrial” application of CMP, it turned out to be an “academic” model, similar to the ones we discussed in the previous section.

2.6 Conclusion

Figure 2.2 summarizes the different categories of models highlighted in this chapter.

We saw that there are a large number of models that employ cutting edge mathematical operations, but are usually limited in their scope. This is sometimes due to their inability to handle complex motion or loading conditions, while in other cases it is because of their extremely high computational cost. These are placed in the category of simpler or academic models.

On the other side are the dedicated industrial models. They are capable of simulating larger length and time scales but sacrifice detail for higher computational speed, critical for realistic engineering design cycle times. These models generally neglect, or employ low accuracy sub-models for effects that are not relevant to that particular industrial application. This means that they are limited to applications

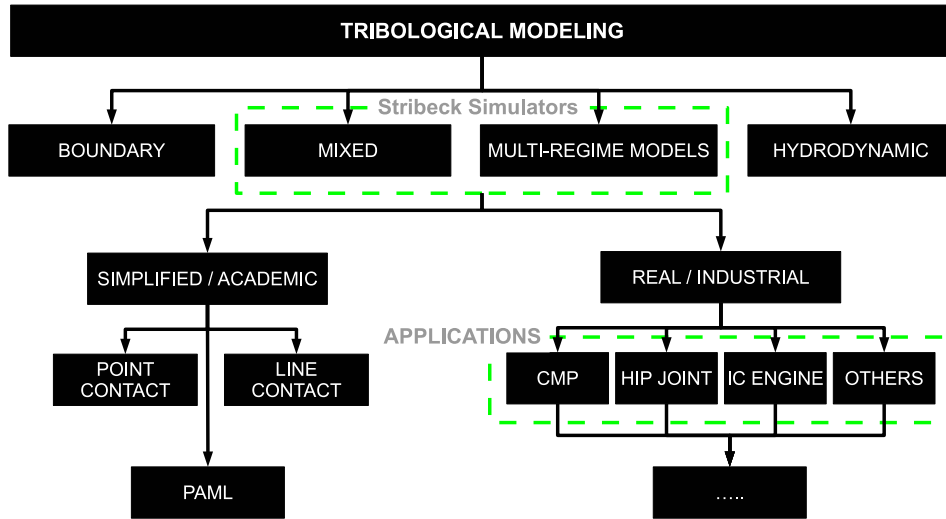


Figure 2.2: Different categories of tribological models geared towards simulating multi-regime behavior

that operate under the same dominant physical phenomena. Moreover, these models also often have empirical or semi-empirical components that further reduce their utility to an even narrower set of conditions.

We can notice that even though there is a large variety of tribological models available for most industrial applications, there has not been any modeling approach that is:

- General enough to be applied to a wide range of tribosystems;
- Accurate enough to act as a replacement, or at least as a guide, to complicated and/or expensive experiments;
- Flexible enough to account for differences in dominating physical phenomena

across tribosystems;

- Computationally efficient enough, to simulate tribosystems with large length and time scales relevant to the industry, in a reasonable period of time

The present work is an attempt at filling this gap by providing a unified (capable of simulating different lubrication regimes), widely applicable modeling framework that can simulate different industrially relevant applications, without sacrificing speed or accuracy.

Chapter 3

The PAML+ Modeling Approach

In the previous chapter we saw that there is a large range of cutting edge models that use the highest fidelity in simulating the tribological behavior of lubricated contacts. However, those high fidelity models were limited in the size of the domain they can simulate, and the motion and loading conditions they can handle. In the other half, we also saw a range of models aimed at simulating industrial applications. But by the end, the previous chapter highlighted the shortcomings of these industrial models that aim to solve problems involving large length and time scales. In those models, the emphasis is on higher computational efficiency, i.e. solving the problems within a reasonable time (in a matter of hours, if not minutes) with modest computational resources (without a massive supercomputer). To achieve higher computational speeds, those models typically neglect one or more major physical interactions, or account for them through empirical coefficients. This, unfortunately, makes them extremely limited in their applicability. Meaning, in simple terms, a model intended for studying journal bearings cannot be used to study the behavior of an artificial hip joint.

At the end of the last chapter, we saw that the objective of the present work is to fill the gap for a general, industrially relevant modeling approach. Again, this research aims to develop a modeling framework that is:

- a. **General:** Can be applied to a variety of applications
- b. **Accurate:** Can match experimental trends qualitatively, preferably quantitatively
- c. **Flexible:** Modular, capable of accounting for all major mechanical interactions
- d. **Efficient:** Can simulate industrially relevant length and time scales and generates results in a reasonable period

To develop a general modeling approach that is capable of simulating a variety of industrial application, it is important to identify the major physical interactions that govern their behavior. While observing major applications one can easily spot four major interactions that contribute most to their performance. These four interactions are discussed in the next section.

3.1 Physics behind the tribology

1. **Fluid Mechanics:** The fluid pressure is the first contributor in the load carrying capacity. In boundary/mixed lubrication, the effect of fluid pressure on the fluid material properties such as density and viscosity is not prominent. However, in the case of EHL, the variations in viscosity and density (in case of compressible lubricants) is significant and needs to be accounted for in the modeling approach.

2. **Solid Mechanics:** In boundary/mixed lubrication regimes, a major part of the load is being carried by the solid-solid contact. Hence appropriate modeling of the elastic deformation under the solid-solid contact stress, or the fluid pressure, is paramount to obtain reasonable predictions from any modeling approach.
3. **Particle Dynamics:** Most of the mixed lubricated interfaces operate under the influence of particles. In some situations, the presence of particles is detrimental to the surfaces as in the case of polishing or teeth wear. In certain other situations, the particles do not directly interact with the tribosystems but still affect the operation of the device, as in the case of the artificial joints whose performance degrade with higher concentration of particles. In all of the cases however, understanding the behavior of particles in mixed lubrication interfaces is of interest.
4. **Wear:** To develop a predictive capability useful to the community, one has to account for the effect of the above interactions on the performance of the device. Wear in majority of the applications is detrimental to the performance, as in the case of piston rings, artificial joints, and teeth degradation. On the other hand, wear is the desired action in the case of the machining operations (polishing, lapping). Therefore, for all models of practical importance, wear is an important deliverable, and must be an essential ingredient of the approach being followed.

Apart from the above four major interactions, depending on the applications, more effects can become relevant and important to explain the tribological behavior. These may include thermal effects as in the lubrication of the internal combustion

engine, or the polishing process; chemical effects, as in the chemical mechanical polishing process; or biological phenomena in understanding the effect of debris transport within the artificial joints or during tooth decay.

3.2 Model Development

The subsequent sections give a brief description of the techniques generally used to model the individual physical interactions in the development of the comprehensive modeling approach. The four objectives mentioned at the beginning of the chapter are to be kept in mind while studying the large range of available options for specific physical interactions.

3.2.1 Solid mechanics

An understanding of the elastic deformation of the bounding solids is of high importance in any tribological application. The finite element method (FEM) is the most common approach applied for high fidelity structural analysis. However, the computational resources required to run even a moderately sized structural analysis are very high. Due to the sharp learning curve, and the difficulty in efficient computational implementation, use of black-box FEM “packages” is widely popular within the research community. These packages however, are very difficult to couple with their user-defined subroutines and interfacing such an FEM based structural solver with an external code is extremely challenging to say the least. Because of these issues with the generally accepted FEM based approach, high accuracy analytical or semi-analytical techniques appear as lucrative alternate modeling tools for calculating elastic deformation in the bounding solids. These approaches do present their own

limitations, primarily the fact that they have limited applicability. The modeler has to find a different analytical technique suitable for every new application. The gains in computational speed and relative simplicity in the computational implementation, far outweigh the effort required to find the correct analytical solution.

3.2.2 Fluid mechanics

Similar to FEM, numerical solution of the Navier Stokes Equation is the standard for computational fluid dynamics (CFD). Unfortunately, the issues that plague FEM are also prominent in the case of the full CFD solution. They require a long tedious process for the development of the solver, and once developed, the computational requirements for such “3-D Navier Stokes solvers” are massive. These issues are more pronounced for tribological applications where the film thickness is several orders of magnitude smaller than the overall dimensions of the system. Because of these concerns, the thin film approximation of the Navier Stokes equations, known as the Reynolds equation, seems useful for the purpose of this work. The Reynolds equation is very useful for tribologists, as its primary output is the fluid pressure. As there is no system of equations to be solved simultaneously, the Reynolds equation is computationally very efficient, as opposed to the 3D Navier Stokes solution. However, to some extent, Reynolds equation is also specific to the application being studied. The variant of the Reynolds equation to be used must be selected based on the coordinate system most suitable for the application.

3.2.3 Particle dynamics

There are two treatments of particle dynamics that are widely popular in the community: Lagrangian and Eulerian treatments. The Lagrangian treatment focuses on

individual particles and provides high resolution information about their position and velocities. The Eulerian treatment approximates the “cloud” of particles as a phase and studies its interaction with the solvent or the fluid phase. Both of these treatments are computationally expensive (Lagrangian more so than the Eulerian), and require coupling with 3D Navier Stokes solution, another computationally expensive technique. Hence, for this approach, statistical treatments would need to be applied to approximate the particle dynamics and their interaction with the bounding solids. In one of the applications, the theory of mass transportation was implemented to model the migration of particles in the interface.

3.2.4 Wear

As mentioned previously, wear is an important quantity for most tribological applications. Since the mechanism of wear can differ significantly between applications, the wear modeling tends to be specific to the application being studied. In some applications, two body adhesive wear is the primary mechanism for material removal. Such a wear mechanism favors statistical treatment which increases computational efficiency, but has added limitations in the form of empirical coefficients. In some other cases, third body abrasive wear dominates all other wear mechanisms, and hence deterministic simulations are needed.

Following the above principles a new modeling framework called *Particle Augmented Mixed Lubrication - Plus*, (abbrv. PAML+) is proposed. Details of the modeling approach are discussed in the next section.

3.3 The PAML+ Modeling Approach

For every application, the PAML+ approach is implemented through the same process, following these steps outlined below.

Fluid Solution

- Step 1 Observe the problem for the dominant motion. Also note the direction along the film thickness. For example, in a journal bearing, even though there is a possibility of radial oscillations in the shaft, the dominant motion is the shaft rotation i.e. in the tangential direction. The film thickness is along the radial direction. Similarly, in a hip joint the dominant motion is along a combination of “inclination” and “azimuthal” direction, and the film thickness is along the radial direction.
- Step 2 Based on the motion and film thickness, select the coordinate system (cartesian, cylindrical polar, or spherical polar). The journal bearing above, should be solved in the cylindrical polar coordinate system, and hip joint in the spherical polar coordinate system. An interesting case here is a ball bearing (fig. 3.1). The film thickness is in the radial direction with respect to the ball which undergoes multi-axial rolling motion over the inner ring. While looking at the ball, the user might be tempted to use the spherical coordinate system. But the dominant motion is along the tangential direction of the inner ring with a radial film thickness, and hence cylindrical polar coordinates is a more appropriate coordinate system.
- Step 3 Pick the appropriate Reynolds equation for the coordinate system chosen in the last step, to solve for the behavior of the fluid. If there is significant

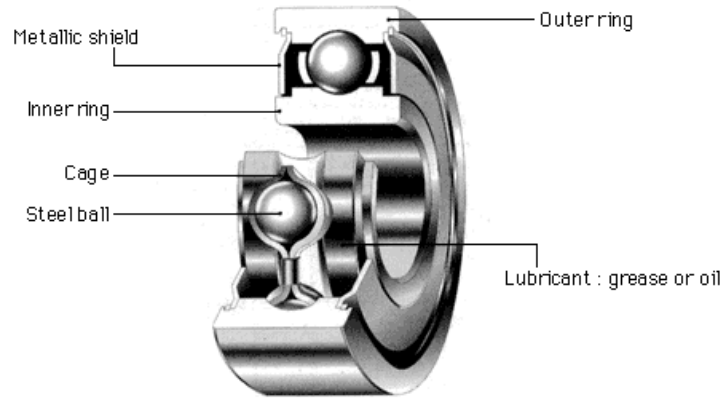


Figure 3.1: Schematic of a ball bearing (ref:www.spb-usa.com)

energy transport, approximate the three dimensional energy equation for thin-film flows, accounting for possible heat sources, such as viscous heat generation.

Solid Solution

Step 4 Since tribological interactions are only affected by the surface deformation of the solids, check if the entire solid deforms, or the deformation can be restricted to the surface only. For that, do the checks given below. Note that, even if the entire solid is undergoing significant deformation, to calculate tribologically relevant quantities such as friction and wear, one only needs to calculate the surface deformations.

Check a: Determine the size of the tribological interface with respect to the solids. If the interface is much smaller than the size of the solid (in the case of a Hertzian point contact, for example), the deformation can be assumed to be in the surface only.

Check b: Compare the stiffness of the “softer” material with the stiffer material. If the softer material is much more compliant than the stiffer material (a difference of at least an order of magnitude between their elastic moduli), the deformation can be limited to the softer material only. Further, if the softer material has a rigid backing, it can be treated as a “mattress”, or collection of springs.

Step 5 If either of Check a: or Check b: are true, the computationally efficient Winkler Elastic Foundation approach can be implemented to calculate the deformation in the solid. If neither of them are true, look for alternative efficient solid treatments, specific to the application. For example, if the solids are in the form of plates, and are experiencing axisymmetric loading, plate theory can be used. Or if the boundary conditions remain roughly constant throughout the simulated period, influence coefficients for surface deformation can be extracted from an FEA package. This is especially useful if thermal effects are significant in the application. Calculating thermo-elastic deformation without FEA is a difficult, and computationally expensive process. If thermal boundaries remain similar over the simulated period, getting influence coefficients for temperature and surface deformations can help retain both accuracy, and speed, in a potentially slow application.

Step 6 Compare the magnitude of the fluid film thickness with the surface roughness. If the fluid film is much thicker than the surface roughness, the system will operate in full-film lubrication regime. If the film thickness is of the same order of magnitude, or smaller than the surface roughness,

partial contact between the surfaces is a possibility. Calculate contact stress using the above mentioned deformation approaches if partial contact exists.

Dynamic Equilibrium

Step 7 Identify the state of equilibrium for the system. Determine which of the six load quantities $F_x, F_y, F_z, M_x, M_y, M_z$ are significant in the system. Determine how the external loads are balanced. If partial contact exists, contact stress together with hydrodynamic fluid pressure provide the required load carrying capacity, as in the case of boundary or mixed lubricated contacts. If no contact exists between the two solids, the loads have to be balanced by the fluid pressure only, as is the case with elasto-hydrodynamically lubricated or hydrodynamically lubricated contacts. In a journal bearing, assuming z axis along the shaft, the load exists in the form of F_x , and F_y only, with all other components negligible. Since there is no partial contact in a journal bearing during operation, the loads are balanced by the hydrodynamic fluid pressure. Similarly, in a hip joint, the body weight acts a three dimensional force vector, and hence F_x, F_y, F_z are non-zero and all the moments are small. Since the hip joint is known to operate in boundary-mixed lubrication regime, partial contact exists and the loads are balanced by both the contact stress and hydrodynamic fluid pressure.

Step 8 Determine the degrees of freedom in the system, along which small movement occurs for the system to achieve a state of dynamic equilibrium.

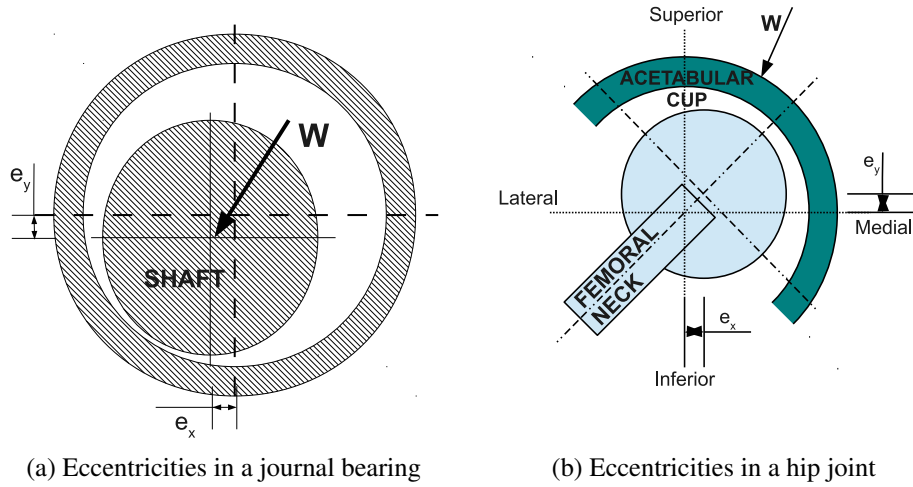


Figure 3.2: The degrees of freedom in a tribosystem. These are quantities that change by a small amount to allow the system to achieve load equilibrium

Generally, if there are force loads, translational degrees of freedom are expected. Rotational degrees of freedom are expected with moment loads. In the case of journal bearing, since there are two force loads, two translational degrees of freedom are observed in the form of shaft eccentricities (e_x, e_y) that allow the forces to be balanced with the hydrodynamic fluid pressure. Similarly, in the case of hip joint three translational degrees of freedom, in the form of three eccentricities (e_x, e_y, e_z) exist that allow generation of hydrodynamic and contact load carrying capacity to balance the body weight.

Post-processing

Once the equilibrium “orientation” (in terms of the degrees of freedom) is obtained, other modes of physics can be added to account for other tribological interactions. Some of the common physical modes are listed

below.

Step 9 Particle Dynamics: Several mixed lubrication applications will be augmented by the presence of particles. In some cases particles aid in lubrication by providing additional load carrying capacity. In other cases, particles act as abrasives and cause surface degradation. In the presence of particles, the following interactions are of interest:

1. **Particle Transport:** Check the size of the particles with respect to the size of the interface. If the particle volume is several orders of magnitude smaller than the volume of the lubricant in the interface, the transport of particles will be much faster than the time scales considered in the simulation. As a result, particle concentration can be assumed to be constant across the entire fluid volume. If particle sizes are larger, there will be a finite, and reasonably small number of particles present in the interface. Discrete element method can then be implemented to study the movement of the particles through the interface, with extremely high accuracy. This would however make the simulation considerably slower.
2. **Particle-Surface Interactions:** If the particles are harder than the bounding solids, they would cause wear on the surface. The material removal can be through two-body wear (as in the case of erosive wear) or third-body wear (as in the case of abrasive wear). If the particles are wear debris from one of the bodies, they can provide additional load carrying capacity by acting similar to the “asperities”. If the particles are attracted towards one of the surfaces, they can get

deposited in the regions where Peclet numbers are low.

Step 10 **Wear:** In case of partial contact, there would always be a possibility of material removal from the softer material. The material removal can get further exacerbated with the presence of the particles. There can be several mechanisms for wear:

- a. **Abrasive wear:** This is the most common wear mechanisms in cases where the third-body material removal is the primary mode of surface degradation. The abrasive particles get trapped in the contact area between the asperities of the two solids. The particles then get dragged along the surface removing material over the distance they slid. Statistical treatments would be required to find out the fraction of particles eventually causing wear, or being “active” particles. Additionally, abrasive wear can also be prominent in two body contacts where one material is significantly harder, and rougher than the other one.
- b. **Adhesive wear:** If the roughness of the two bodies in a two-body contact are of the similar orders of magnitude, adhesive wear would be the primary mode of material removal. Also, if there is two body contact between bodies of the same, or similar materials (metal-metal, polymer-polymer etc.) adhesive wear would again be the dominant material removal mechanism. The wear volume can then be calculated by using the load, sliding distance, material hardness and an empirical wear constant.
- c. **Erosive wear:** The most common mode of erosive wear is particle

based erosive wear, where particles impinge on the surface with kinetic energy higher than the surface energy. The particles then impart that kinetic energy to the body which causes severe plastic deformation on the surface and results in wear debris being generated. In tribology, the fluid film thicknesses are very low, fluid viscosities high, and velocities relatively low, the particles do not achieve velocities high enough to cause erosive wear in most systems. Still, statistical treatments based around the fluid velocity can be implemented to approximate the erosive wear volume.

- d. There are other wear mechanisms present in specific applications, such as corrosive wear in the presence of chemicals, or fatigue in cyclic motion, or fretting wear as a combination of both. All of these wear mechanisms can be implemented in the approach once the equilibrium orientation for the tribosystem is known.

Step 11 The above analysis can then be repeated over several time-steps if the problem being studied requires transient analysis.

3.4 Applications

Following the “objective” mentioned at the beginning of the chapter, this approach is aimed at solving a large variety of industrial problems. To demonstrate the strength and predictive capabilities of the PAML+ approach, four major tribological problems were modeled with this approach. It should be noted that for each problem, the author developed fairly deep experiential learning on the problem through industrial collaboration, summer internships, and advanced topic classes with experts in the

field. The goal was to ensure that the modeling approach treated the most difficult physical interactions of the problem, thereby providing answers that other single-regime tribology models could not. Four specific applications tackled as a part of this work were:

1. Pin-on-disk tribometry (Fig. 3.3a)
2. Chemical mechanical polishing (Fig. 3.3b)
3. Artificial hip joints (Fig. 3.3c)
4. Mechanical seals (Fig. 3.3d)

One can notice however, that with a comprehensive modeling approach that has the flexibility to account for all major physical interactions with sufficiently high fidelity, *any* tribological application can be modeled. Beyond the applications above, other examples of tribology problems that do not necessarily operate in the mixed lubrication regime, but can still be studied using the current approach, are given below:

- *Hydrostatic thrust bearings*: Hydrostatic thrust bearings, as the name suggests, operate in the hydrostatic lubrication regime, driven by an external pumping source. The hydraulic pressure generated in the fluid provides the load carrying capacity. An approach, with a comprehensive fluid modeling component can easily calculate the pressure distribution within the interface, and the resulting load carrying capacity and can hence predict the performance of such a bearing.
- *Squeeze film bearings*: Squeeze film bearings are generally employed in applications where the motion of the bounding solids, which is often oscillatory



Figure 3.3: Applications studied through the PAML+ approach in this work

in nature, is in the direction normal to their interacting surfaces. The load carrying capacity is generated by squeeze resistance of the fluid. A modeling approach that accurately calculates the fluid pressure in the case of normal motion of the bounding solids, can easily model the behavior of thrust bearings.

- *Deposition of a transfer film:* A presence of self replenishing transfer films

facilitates lubrication when using powder lubricants. A source of soft, slippery powder, usually in the form of pellets is used as a sacrificial component in such applications. A modeling approach that is capable of calculating the contact stress between the pellet and the workpiece, and the resulting material removal, can predict the behavior of this powder lubricated tribosystem.

3.5 The Model's Name: PAML+ instead of PAML-lite

The framework's name was originally called "PAML-lite" because it was developed to extend the length and time scales of the original PAML model [61] while still being computationally efficient. The intent was to be able to tackle tribological applications at the scale of both the first bodies that are in a lubricated contact, and capture the real interface between them. It was thought that since simplifying assumptions were used, it was actually a "lighter" model, and hence was named "PAML-lite". However reviewers of one of the author's paper [62] (Chapter 5 in this thesis) commented how the name "lite" took away some of the merits of the model. And since the model really extended the PAML type approach to more engineering problems and more of the interface (i.e. larger length scales), the framework was retitled, from "PAML-lite" to "PAML+".

Part II

Applications of the Modeling Approach

Chapter 4

Applications: A Textured Pin-on-disk Tribosystem Model

4.1 Introduction

Total hip replacement has been referred to as the operation of the century, after its wide acceptance in the 1960s provided for the ability to drastically increase the agility and comfort of both elderly patients and also of younger, more active patients with early onset hip problems [1]. The distinctive features of the joint are the acetabular cup, often metallic or polymeric, and the femoral head which is often a harder ceramic or metallic alloy. The joint itself is lubricated by synovial fluid with experimentally determined, shear-thinning viscosities between 0.0025 and 0.0009 Pa-s, which are relatively low compared to common industrial lubricants but close to water [?]. While walking, the hip joint interface experiences a combination of normal loading and surface tractions, which are often approximated as locally sliding contact between surfaces. The actual loading conditions were estimated by

Dowson, who reported average loads of 1346 N and average sliding speeds of 1.5 rad/s for the normal gait cycle [?]. Alternatively, in the work of Hodge et al., contact pressures were captured in vivo and found to vary between 1-10 MPa, also during the gait cycle [63]. Many authors have presented different mechanisms for the ongoing tribological interactions in the artificial hip joint. Because of the relatively high load, low speed, and low viscosity sliding contact, the lubrication exists primarily in the boundary and mixed lubrication regimes where the load is borne by a mixture of fluid-surface and surface-surface asperity contact. As a result, only occasionally are speeds and pressures developed which are sufficient for full film separation of the surfaces. In addition, with progressive use, the lubricant can become filled with particulate debris, thereby putting the interface into what the authors refer to as a particle augmented mixed lubrication regime. In this special case, it has been shown that the presence of particles in the interface significantly alters the lubricating performance, most commonly by accelerating the abrasive wear process. Given the added complexity of these problems, numerical modeling approaches are generally used to capture the interplay between the fluids, particles, and surfaces. In the presence of these more severe lubrication regimes, total hip replacement has been plagued with unacceptable clinical lifespans due to premature failures, reducing average joint life from an expected 50 years to just 12 years [64,65]. The primary cause of these failures was found to be a number of harmful effects, incited by excessive abrasive wear and debris generation at surface-surface contacts. These effects include granulomatosis lesions and osteolysis, which lead to bone resorption, pain, and aseptic loosening of the prosthesis.

In non-biomedical applications, surface texturing has been shown to promote low-wear, low-friction sliding contacts [10-17]. In these works, the textures are

typically fabricated through a process known as laser surface texturing (LST), in which dimples are created by a concentrated laser pulse. While proving to reduce friction in dry and lubricated contacts, this technique has thus far been implemented primarily with seals and automotive piston rings. The advantages of surface textures are considered to be: (i) micro-traps for collecting unwanted wear debris from the sliding contact, (ii) lubricant reservoirs that enhance hydrodynamic pressure and facilitate the onset of full-film hydrodynamic lubrication, and (iii) solid lubricant reservoirs for in situ replenishment, which is less relevant, as of yet, to the current work. Although abrasive debris generation in current artificial hip joints prevents long-lasting single surgery replacement, this work proposes that surface texturing may provide a solution through its ability to control friction and wear. In terms of hip joint materials, work already exists in which artificial roughness, created through a water jet erosive wear process, was shown to trap UHMWPE wear debris. While this approach may be useful to mitigate the problems of existing wear debris, including its self-exacerbating effects, a more complete approach would involve utilizing the pressure enhancing effects as well. Although wear trapping may limit the adverse effects of interfacial wear debris, the hydrodynamic pressure enhancing effects can help to mitigate debris generation in the first place. Therefore, this work will seek to take a more deterministic approach for creating precisely controlled, dimpled surface textures on hip joint materials. The goal is to conduct a study to explore the merits of texturing, namely the assessment of the aforementioned first and second advantages under realistic loading conditions that typify human walking.

4.2 Modeling Scheme

The philosophy of the proposed modeling scheme has two parts: determining the quasi-equilibrium configuration of the pin over the disk, and, calculating the net friction and material removal in that configuration. The state of quasi-equilibrium is achieved when the net force acting on the pin vanishes. Due to circular symmetry in the process, the net horizontal force (in X and Y directions) is assumed negligible. For the same reason, the vertical moment (in Z direction) is also neglected in the present analysis. Moreover, the mechanism to mount the pin in most traditional tribometers restricts horizontal moments (in X and Y directions). As a result, the only load that needs balancing is the force along the vertical (Z-axis). The major forces acting on the pin during a test are the hydrodynamic pressure of the lubricant, the compressive stress due to partial contact with the disk, viscous shear stress from the lubricant, friction due to relative sliding with the disk and lastly, the applied normal load. Of these, the normal forces, i.e. the fluid pressure, the contact stress and the applied load are used to evaluate the force balance. And the tangential forces, viscous shear stress and sliding friction are used to calculate the effective coefficient of friction. The lubricant is assumed to behave as an incompressible and Newtonian fluid, and the disk is assumed to be made of a linear-elastic and isotropic material. Based on these assumptions, a comprehensive model is presented here that accounts for the effect of the fluid lubricant, solid-solid contact between the pin and the disk, and possible wear due to relative sliding between the pin and disk asperities. The following sections describe the major components of the model.

4.2.1 Hydrodynamic (lubricant) modeling

In the presented model, the hydrodynamic pressure acting on the pin plays an important role in determining the equilibrium orientation of the wafer. The Reynolds Equation has been used to calculate the hydrodynamic pressure acting on the wafer surface. Following the rotational symmetry of the interface, the Reynolds Equation obtained using 3D Navier Stokes equations in cylindrical coordinates, has been implemented [66].

$$\begin{aligned}
 & \frac{1}{12\eta} \left[\frac{\partial}{\partial r} \left(rh^3 \frac{\partial p}{\partial r} \right) + \frac{\partial}{r \partial \theta} \left(h^3 \frac{\partial p}{\partial \theta} \right) \right] = \\
 & -rv_{r(p)} \frac{\partial h}{\partial r} - v_{\theta(p)} \frac{\partial h}{\partial \theta} \\
 & + \frac{\partial}{\partial r} \left(\frac{v_{r(d)} + v_{r(p)}}{2} rh \right) + \frac{\partial}{\partial \theta} \left(\frac{v_{\theta(d)} + v_{\theta(p)}}{2} h \right)
 \end{aligned} \tag{4.1}$$

The primary quantity dictating the fluid pressure (p) in the Reynolds Equation (eq. (4.1)) is the film thickness h . The film thickness in this model has been approximated as the separation between the mean planes of the pin and disk asperities (Fig. 4.1). To avoid singularity, elements where h approaches 0, are excluded from the domain of solution of the Reynolds equation.

The velocities have been calculated with the pin's axis of rotation as the origin (Fig. 4.2). Equation (4.1) above is a more general form of Reynold's equation with both solids rotating about their own axes. However, in this case, the rotation of the pin about its axis has been neglected ($\Omega_{pin} = 0$ in eq. (4.2)), which results in further

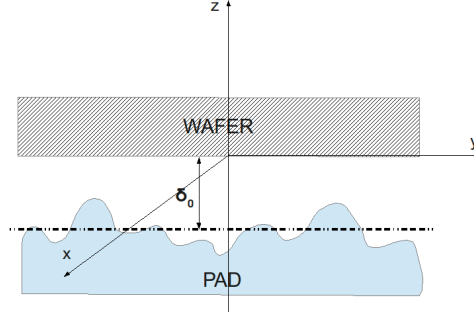


Figure 4.1: Film thickness is assumed to be the mean separation between the pin and the disk

simplification of eq. ((4.1)).

$$v_{r(d)} = r_{pd} \sin \theta \Omega_d \quad (4.2a)$$

$$v_{\theta(d)} = (r + r_{pd} \cos \theta) \Omega_d \quad (4.2b)$$

$$v_{r(p)} = 0 \quad (4.2c)$$

$$v_{\theta(p)} = r \Omega_{pin} \quad (4.2d)$$

4.2.2 Pin-disk contact

In the setup being used, the disk is made of a polymeric material placed on top of a rigid metallic platen. The pin used is made of a metallic material (typically SS304), and is much tougher than the polymeric disk. Figure 4.3 shows the different geometries of pins used in the simulations. The solid-solid contact between the pin and the disk can be modeled through a Winkler Elastic Foundation [67] which approximates the softer material as a mattress, constructed by assembling a set of

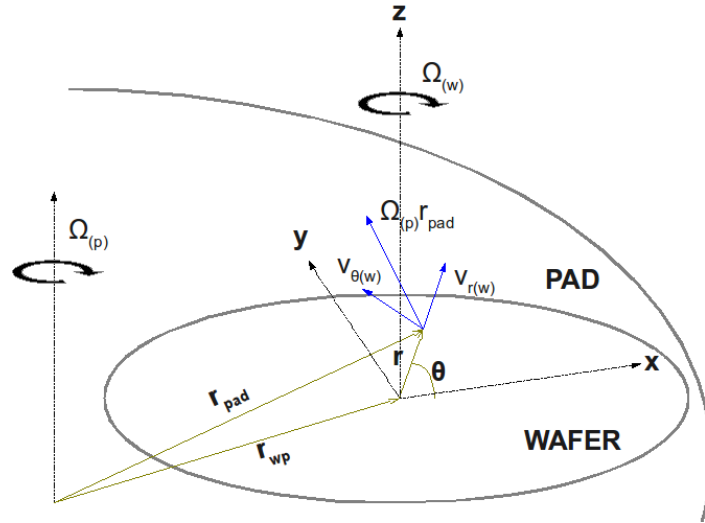


Figure 4.2: Different velocities in the system

parallel springs. In this case, each spring represents a collection of, or a single asperity, occupying a rectangular area, and representing the average height of that area. It is assumed that these springs deform vertically, without influencing their neighbors. This provides a relationship (eq. (4.3)) between the stress and normal deflection for each spring, as has been described by Johnson [Johnson(1985)]

$$\sigma(x,y) = K \frac{u(x,y)}{\Delta} \quad (4.3)$$

Here σ is the contact pressure, Δ is the initial height of the mattress, and u is the surface deflection. The following assumptions were made to determine the proportionality constant:

- Tangential deflection of the asperities is neglected
- The effect of the tangential loads on the normal deflection is neglected

With the above assumptions, the equations of elasticity for the pad can be condensed to eq. (4.4)

$$\sigma(x, y) = \frac{E_{disk}(1 - \nu_{disk})}{(1 - 2\nu_{disk})(1 + \nu_{disk})} \frac{u(x, y)}{\Delta} \quad (4.4)$$

This expression explicitly relates the normal stress $\sigma(x, y)$ to the normal deflection $u(x, y)$ of an asperity. As a result, the calculation of contact pressure can be obtained through $O(N)$ operations, which is critical to maintain the speed and memory efficiency of the model.

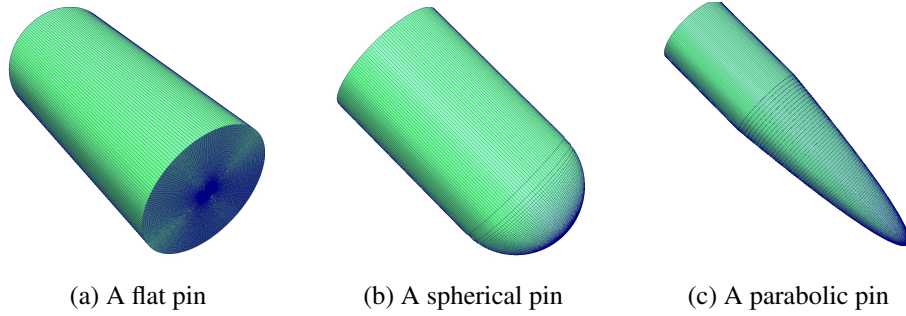


Figure 4.3: Different pin geometries used in the simulations

4.2.3 Equilibrium Orientation

The fluid and contact pressure fields are used to formulate the load balance equation with the nominal clearance (δ_0) as the independent variable. The constructed equations is a non-linear, implicit equations, and hence it is not possible to obtain an analytical solution. Root finding method based on the bisection algorithm has been implemented to solve the equation. It is important to note that the equilibrium being discussed here, is a quasi-steady equilibrium. As the disk rotates, the topography interacting with the pin changes, thus modifying the hydrodynamic pressure and the contact stress field. For the new sets of pressure fields, a new equilibrium orientation

appears, and this process is repeated at every time step.

4.2.4 Friction

The net shear resistance to sliding in the interface has two components. The first is from the kinetic friction between the pin and disk. It can be determined by using the contact stress that (together with the fluid pressure at that value of δ_0) balances the load (eq. (4.5a)). The second is from the viscous shear stress acting on the surface of the pin due to the entrainment of the lubricant in the pin-disk interface. This is determined by using the couette-poiseuille velocity profile that is in turn governed by the equilibrium pressure distribution (eq. (4.5b)). The net friction force is calculated by obtaining a vector sum of these two components (eq. (4.5c)).

$$\tau_s(r, \theta) = \mu_k \sigma(r, \theta) \hat{\mathbf{n}} \quad (4.5a)$$

$$\tau_f(r, \theta) = -\eta \frac{\partial \mathbf{v}}{\partial z}(r, \theta, z = pin) \quad (4.5b)$$

$$\mathbf{f} = \int_A (\tau_s(r, \theta) + \tau_f(r, \theta)) dA \quad (4.5c)$$

4.2.5 Wear

In a pin-on-disk setup, in the absence of any third bodies or abrasive particles, there can be two possible mechanisms of wear:

1. Abrasion of the softer, disk material by the tougher asperities of the pin
2. Adhesive contact between the pin and disk surface resulting in adhesive material removal from the disk

The disk material being used is highly crosslinked Ultra-High Molecular Weight Polyethylene (HXL UHMWPE), which is considered to be one of the most abrasion resistant materials. Considering this, adhesive wear is assumed to be more prominent wear mechanism. With that assumption, the material removal is assumed to follow Archard's wear law [?]:

$$\Delta M = K_{wear} \frac{F_n v_{rel}}{H} \quad (4.6)$$

Here, F_n is the applied normal load, v_{rel} is the relative sliding velocity, H is the hardness of the softer material and K_{wear} is the wear constant that is obtained from the experiments.

4.3 Experiments

4.3.1 Experimental setup

A Bruker UMT-3 tribometer (Fig. 4.4) was used to monitor the tribological behavior of the interface. The tested materials included disk specimens, which were made out of textured and un-textured UHMWPE, and pin specimens made of stainless steel. It is worth mentioning that in the future, texturing of the harder femoral head component would be more advantageous. In any tribological system, the metallic component is less likely to deform or wear. This would result in the textures retaining their shape for a longer time, and yield longer lasting performance enhancement. In this case, the UHMWPE disk was chosen as the texturing surface solely for its lower fabrication cost. In order to best capture the ability of textures to enhance the lubrication effectiveness, tests were conducted in which the speed was ramped up after discrete time intervals. These speeds were varied between

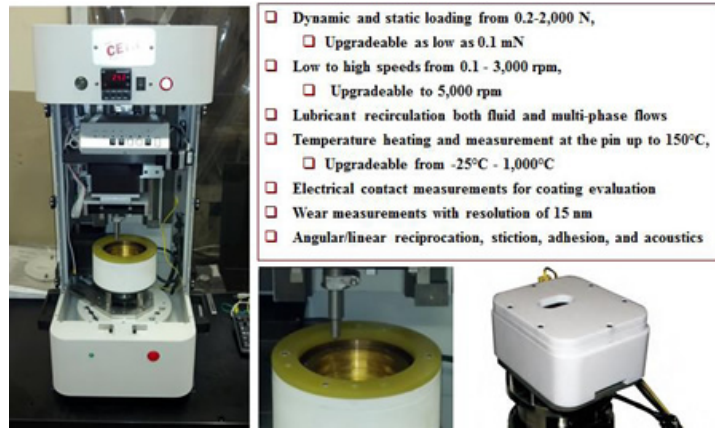


Figure 4.4: Bruker UMT-3 tribometer used for the experiments

5-70 mm/s to simulate typical conditions in an artificial hip joint (average speed close to 20 mm/s is observed during normal walking), while the loads were kept constant for a given test. An average friction coefficient was calculated at each interval for the current speed, so that a Stribeck curve could be plotted for each test. The common lubricant across all tests was water, which is known to have dynamic viscosity similar to the synovial fluid present in human joints. The interface was kept flooded through the use of the UMT's lubricant recirculation system to ensure sufficient lubricant supply.

4.3.2 Surface texturing

As opposed to traditional laser surface texturing (LST) or abrasive water-jet (AWJ) erosion, the surface textures for this study were created through a technique known as micro-machining, using a high precision five-axis micro-machining tool. This technique was chosen not only for its low-cost, but also for its precision and control over the dimensions and shapes of the textures. These were added benefits over

Table 4.1: Texture dimensions

Sample	Approximate Texture Depth (μm)	Approximate Texture Width (μm)
Sample 1	N/A	N/A
Sample 2	10	100
Sample 3	20	200
Sample 4	30	300
Sample 5	40	400

the other techniques such as the AWJ which needs extensive calibration to the given material or even LST which has the risk of heat affected influencing the results. For this work, recessed spherical textures were created using different size ball-end micro-endmills at varying penetration depths to arrive at desired aspect ratios (dimple depth/dimple width). As a first approach, the aspect ratios were maintained at an average value of 0.1, which was found to exist in an optimal range in prior texturing experiments for pistons and seals. The texture dimensions of each tested sample are listed in Table 4.1. A constant texture per area value of about 4 textures per mm^2 was maintained, and separation between textures was appropriately adjusted.

4.4 Results

The Reynolds equation was numerically solved through finite differencing on a grid with resolution such that each dimple was formed by at least 10 elements in both radial and tangential directions. The half-sommerfeld boundary condition was used to account for cavitation of the lubricant in sub-ambient pressure region. Table 4.2 shows the various input parameters used in the model.

Table 4.2: Model Parameters

disk Properties	
disk material	UHMWPE
Elastic Modulus (Bulk)	720 MPa
Elastic Modulus (Tip)	1.1 GPa
Poisson's Ratio	0.4
Hardness	70 MPa
Asperity Distribution	Gaussian
Thickness	4.0 mm
Roughness	1 μm
Pin Properties	
Elastic Modulus	110 GPa
Poisson's Ratio	0.16
Hardness	2.0 GPa
Asperity Distribution	Gaussian
Roughness	1 μm
Lubricant Properties	
Solvent	Water
Solvent density	1000 kg/m ³
Viscosity	0.001 Pa-s

4.5 Load Carrying Capacity

To demonstrate the capability of the PAML-lite modeling approach to seamlessly transition from boundary to mixed to hydrodynamic lubrication regimes, a “Stribeck” test was conducted on the contact between a textured disk and a flat pin. The Sommerfeld number ($= \frac{\text{Viscosity} * \text{Velocity}}{\text{Load}}$) was increased and contact stress and fluid pressure were monitored to observe the transition from boundary, or full contact, to mixed, or partial contact, to hydrodynamic, or full film lubrication. Figure 4.8 shows the progression of contact stress as the Sommerfeld numbers increase from a

minimum value of about 4×10^{-6} to a maximum value of about 78×10^{-6} . At high load, low velocity conditions, characterized by lower Sommerfeld numbers, it can be seen that the entire surface of the disk (the area outside the dimples), is in contact with the pin. This is similar to Stage E shown in fig. 1.2e. As the load decreases and velocity increases, reflected as an increase in Sommerfeld number, the solid-solid contact stress reduces. Moreover, as the Sommerfeld number increases, lesser and lesser disk asperities are in contact with the pin, representing Stage D in fig. 1.2d. As the Sommerfeld number reaches the maximum value studied there are very few asperities still in contact, and those too have virtually no contact stress. The load is almost entirely supported by the fluid pressure. This represents Stage C, as in fig. 1.2c. This demonstrates that with modifying load, velocity and fluid viscosity, the model is able to traverse multiple lubrication regimes, similar to an experimental Stribeck test.

4.5.1 Parametric Results

To compare the effect of texturing the surface, a parametric study was conducted at 10N normal load with water as the lubricating fluid, comparing a textured disk against an un-textured one. The effect of varying the texture size was also studied. The Stribeck behavior of each disk is studied by plotting the variation in the average coefficient of friction (COF) with increasing speed. Generally, the Stribeck curves are plotted in dimensionless parameters (COF vs Sommerfeld Number). But here, for the sake of simplicity, the COF is plotted against the velocity of the disk, which if the load and viscosity are held constant, represents the variation in the Sommerfeld number.

Friction Measurement

Figure 4.5 shows, the experimental measurements conducted for different samples. It can be seen that the textured disk outperformed the un-textured samples at all speeds. For the un-textured case, it is expected that the contact exists only in the boundary lubrication regime even at the highest speeds, indicated by higher COF and a lack of any decrease with increasing speed. The textured cases, however, display a much different trend. For the widest dimple of 400 μm , one can observe that the friction begins with a similar increasing trend, almost touching the un-textured curve at a speed of 20 mm/s and a COF of about 0.076. For such wide textures, it is likely that the solid-solid contact area is smaller than the texture itself, which would negate the lubrication enhancing benefits of the texture at lower speeds. However, a clear transition was discovered at 20 mm/s, eventually decreasing the final COF to just above 0.04. This marked decrease, which begins to level out at higher speeds, suggests that the surface texture effectively shifts the operational mode from boundary to mixed lubrication regime. For the smallest dimple width of 100 μm , a similar trend is noticed, but it appears that even at low speeds of 5 mm/s the operation may already be in the mixed lubrication regime. Transition can again be observed albeit at a lower rate, down towards a similar minimum COF value near 0.04. It is found that a dimple width of 200 μm , which is an intermediate value, provides the lowest and flattest COF. For this dimple width, the COF begins and remains almost constant, at the low value of 0.04 even at the low speeds of 5 mm/s. One can hypothesize that the interface achieves the hydrodynamic lubrication regime at much lower speeds ($< 5\text{ mm/s}$).

Similar observations can be made with the predictions from the model. As

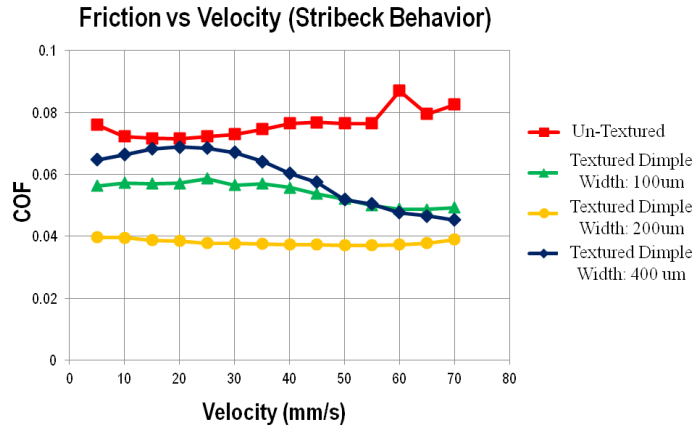


Figure 4.5: Experimental measurements of friction with increasing speed for several disk samples. All textures perform better than an untextured disk, with an intermediate texture size (and neither extreme) resulting in optimum performance.

Fig. 4.6 shows, the textured discs again perform better than the un-textured disk at all velocities. Although the magnitudes of friction coefficients are not similar, trendwise similarity is evident. Once again, textures with size of $200\mu\text{m}$ can be seen to perform best of the samples studied.

Wear Measurements

Wear predictions were made for different texture dimensions mentioned earlier. The model predicts that the texture size of $200\mu\text{m}$ gives the least wear volume. This coordinates well with the frictional behavior as the $200\mu\text{m}$ texture had the lowest friction coefficient as well. The $200\mu\text{m}$ texture transitions away from boundary to mixed lubrication regime sooner than the $300\mu\text{m}$ texture, and much sooner than the untextured sample which has the highest amount of wear, possibly because of high levels of solid-solid contact. This also shows that the wear performance of surface textures does not follow a monotonic trend. Large size textures can have

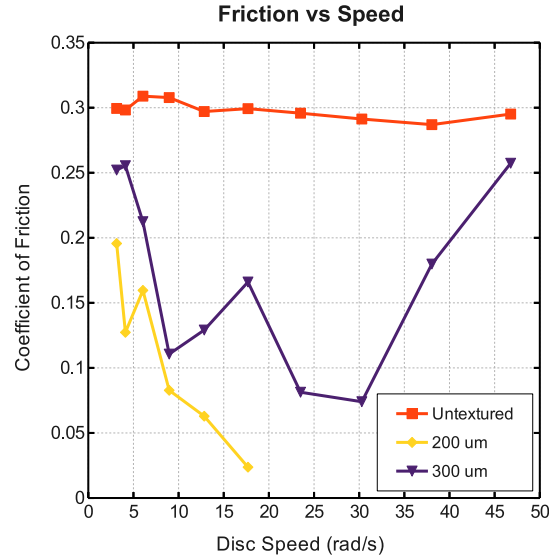


Figure 4.6: Model predictions of friction with increasing speed for several disk samples. Similar to experiments, here both textures performed better than the untextured sample. Also, the lower texture dimension had a better frictional performance.

detrimental effects too.

4.5.2 Model Limitations

The biggest limitation of the model lies in its inability to seamlessly unify the three distinct lubrication regimes: the dry lubrication regime, the mixed lubrication regime, the full film lubrication regime. Although Fig. 4.8 represents a drop in contact stress upon increasing Sommerfeld number, full lift-off conditions (i.e. zero contact stress under the entire pin) are not observed even for the highest Sommerfeld numbers. The load sharing criterion between the fluid and solid would need improvement, and can potentially lead to better prediction of Stribeck behavior.

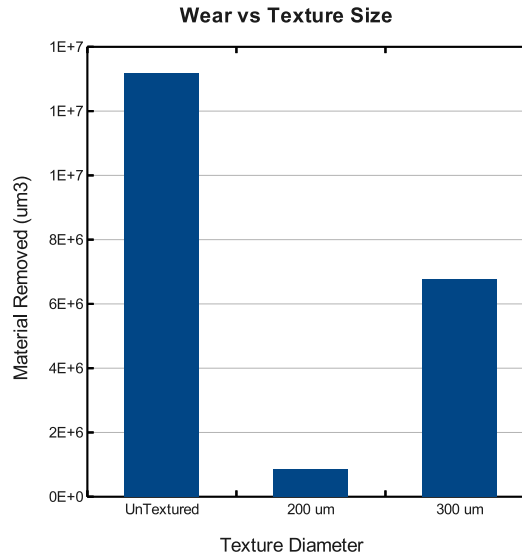


Figure 4.7: Model predictions of cumulative wear for several disk samples. An intermediate texture size ($200\mu m$) results in lowest amount of wear.

Another limitation is the wear model. The wear mechanism for this setup has been implemented as a semi-empirical wear law. Physics based wear modeling would allow further insights into the behavior of the tribosystem during the dry and mixed lubrication regimes.

4.6 Conclusion

A new multi-physical modeling framework is presented to simulate a typical pin-on-disk tribosystem. A stationary pin is pressed against the rotating disk with a vertical load. The disk is preferentially textured in the shape of spherical dimples.

Over a Stribeck test that observes the interface while increasing the Sommerfeld

number = $\frac{\text{Viscosity} \cdot \text{Velocity}}{\text{Load}}$ the model demonstrated the capability to transition seamlessly from boundary or dry lubrication regime, through different stages of mixed lubrication regime, to the hydrodynamic or full film lubrication regime.

The frictional response at the pin-disk interface is also monitored. The model trends match qualitatively with experiments conducted in a Bruker UMT3 tribometer which measures friction *in situ*. Wear volumes predicted by the model also correspond well with frictional behavior. Through the model predictions, and experiments, it can be observed that frictional and wear performance of surface textures does not follow a monotonic trend. An intermediate texture size had the best frictional response, and generated least amount of wear debris. For best performance, the texture design needs to be optimized through an experimental or numerical tool.

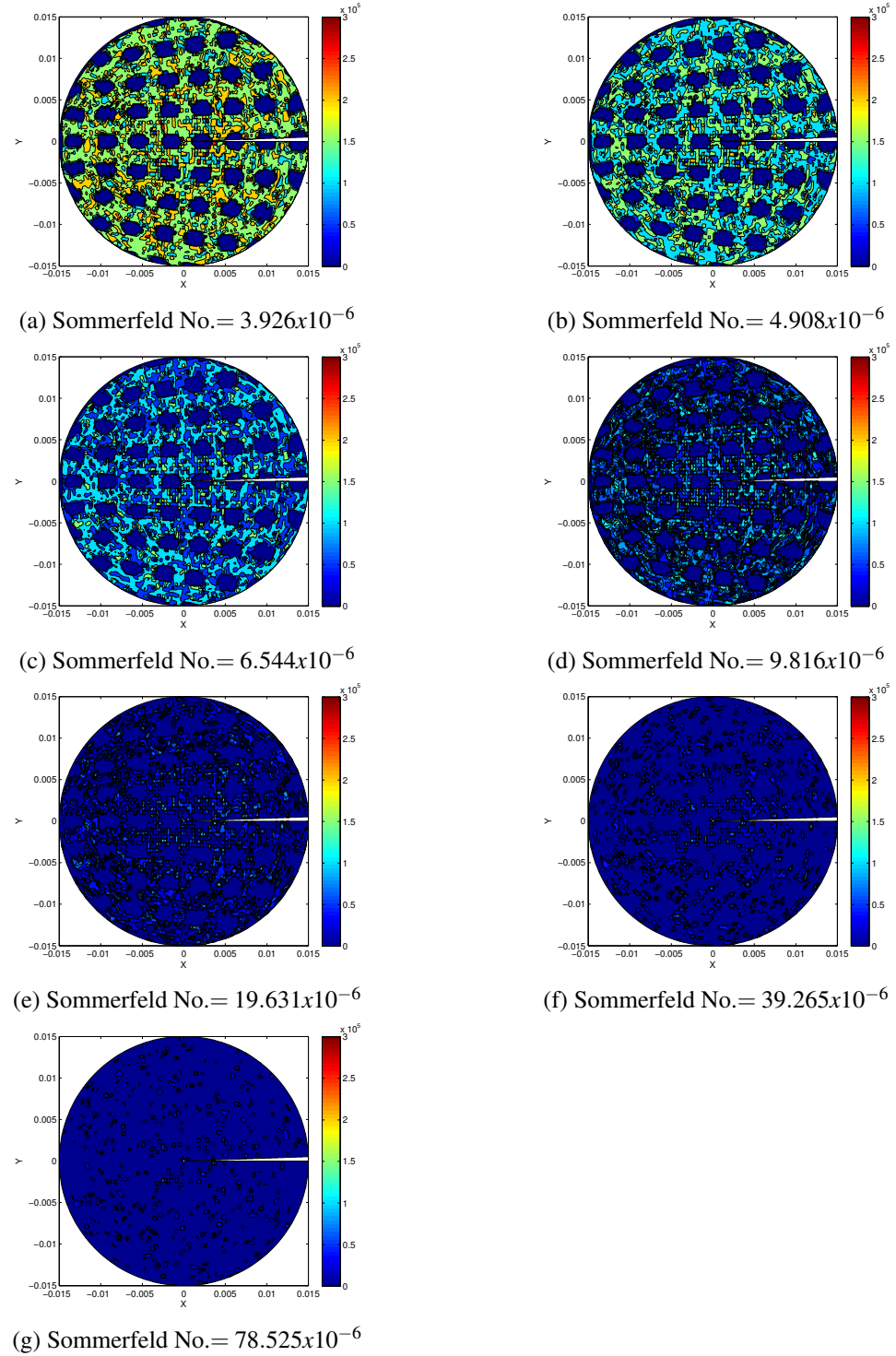


Figure 4.8: Contact stresses in a contact between a flat pin and a textured disk, for several Sommerfeld numbers. As the Sommerfeld number increases, the system moves from dry, or full contact, through different stages of mixed lubrication (fig. 1.2), to hydrodynamic or full film regime

Chapter 5

Applications: Chemical Mechanical Polishing Model

Note: The model described in this chapter has been filed as an intellectual property by Carnegie Mellon University (CMU). Any for-profit use of the modeling approach described herein requires contacting the CMU Center for Technology Transfer and Enterprise Creation (CTTEC)

5.1 Introduction

Chemical mechanical polishing has been a critical process for achieving surface planarization in electronics, and is commonly used as an intermediate fabrication step for devices such as integrated circuits [68], light emitting diodes [69, 70] and magnetic hard disk read/write heads [71]. Although CMP is a common practice in the precision manufacturing industry, the tribological mechanism of the process

is not completely understood. This is primarily due to the complex nature of the interactions between the wafer, pad and the abrasive particles.

Several models have been proposed to explain the wear action in the CMP process, ignoring one or more of the physical phenomena involved. Some of the earlier studies presented empirical models based on results from CMP experiments. Preston in his landmark paper [3] presented the first mechanical model relating the material removal rate to the work done by the frictional force. This approach though reasonable under certain restrictions, does not reveal insights into the wear mechanism. Zhao and Chang [72] and Luo and Dornfeld [73] published seminal wear models based on the real contact area between the pad and wafer interface and the calculation of active particles. Both models gave an accurate fraction of "active" particles, as shown by [74], thus resulting in reasonable wear prediction. However, both of them acknowledged the fact that the slurry flow behavior would play an important role in the polishing mechanism, something that both models neglected. Another group of authors such as Sundararajan et al. [75] have approached CMP with fluid hydrodynamics to calculate wear by calculating the hydrodynamic pressure. Their models, as opposed to the previously mentioned category of models, captured the behavior of the slurry quite well, but ignored the effect of contact between the pad and wafer surfaces, thus neglecting the possibility of abrasive wear. The final approach builds up on the theories of contact mechanics and fluid hydrodynamics. Shan et al. [58] presented a one-dimensional model to predict interfacial fluid pressure under the wafer by solving an average flow Reynolds Equation by introducing mixed-lubrication (the lubrication process where the load is being carried by the fluid, together with a solid-solid contact) into CMP. Higgs et al [?] extended that

work to two dimensions with a stationary wafer and determined the equilibrium orientation for calculating the hydrodynamic pressure and contact stress. Similar work was done by Jin et al. [60] following the theory of elasto-hydrodynamic lubrication. However, the seminal EHL or mixed lubrication studies for CMP were just oriented towards predicting the interfacial lubrication process and did not address the material removal aspect of CMP.

All the approaches mentioned above were set up at the wafer-scale and did not predict the presence of defects at feature scale, namely dishing, erosion and micro-scratching. Identifying a phenomenon they called particle augmented mixed lubrication (PAML), Terrell and Higgs [61] presented an asperity scale deterministic model that can overcome these shortcomings of the wafer-scale modeling approach. However, due to the high computational costs, even with a small domain, the model was still computationally quite expensive. The present study similar the earlier PAML study, integrates the effect of slurry fluid flow, the mechanics of wafer and pad contact, and includes abrasive wear of particles for the process of polishing. The approach here, is presented as a wafer-scale analysis, intended to capture the wafer-scale defects such as inter-die polishing differences.

5.2 Modeling Scheme

The philosophy of the proposed modeling scheme has two parts: determining the quasi-equilibrium orientation of the wafer over the polishing pad, and calculating the material removal in that orientation. The state of quasi-equilibrium of the wafer is achieved when the net forces and moments acting on the wafer, vanish. Due to apparent circular symmetry in the process, the net horizontal force (in X and Y

directions) is assumed negligible. For the same reason, the vertical moment (in Z direction) is also neglected in the present analysis. As a result, the only conditions required to satisfy, for dynamic equilibrium are $F_z = 0$, $M_x = 0$ and $M_y = 0$.

The major forces acting on the wafer during CMP are the hydrodynamic pressure applied by the slurry, the contact pressure applied by the pad asperities, the frictional resulting from the contact pressure and the external load applied on the wafer carrier. The slurry flow is assumed to be incompressible and Newtonian and the pad material is assumed to be linear-elastic and isotropic. Based on these assumptions, a comprehensive model is presented here that accounts for the effect of the slurry, solid - solid contact between the wafer and the pad, and wear due to the abrasive particles in the slurry. The following sections describe the major components of the model.

5.2.1 Hydrodynamic (slurry) modeling

The effect of the slurry on CMP has been widely acknowledged previously, even by the authors who excluded the slurry from their models [72, 73]. Some authors have claimed that the chemical erosion is the dominant material removal mechanism in CMP and have hence focused their entire approach towards accurate prediction of the hydrodynamic behavior of the slurry [75, 76].

The authors of the present study also acknowledge the effect of the slurry on the polishing process, and have thus integrated the effect of the slurry as an important part of the analysis. In the presented model, the hydrodynamic pressure acting on the wafer plays an important role in determining the equilibrium orientation of the wafer. Similar to previously mentioned studies [?, 58, 75], the Reynolds Equation has been solved to calculate the hydrodynamic pressure acting on the

wafer surface. Due to the cylindrical geometry of the interface, the cylindrical polar form of Reynolds Equation (eq. (A.1)) given by Beschorner and Higgs [66] has been used in the current model.

$$\begin{aligned}
& \frac{1}{12\eta} \left[\frac{\partial}{\partial r} \left(rh^3 \frac{\partial p}{\partial r} \right) + \frac{\partial}{r \partial \theta} \left(h^3 \frac{\partial p}{\partial \theta} \right) \right] = \\
& - \quad rv_{r(w)} \frac{\partial h}{\partial r} - v_{\theta(w)} \frac{\partial h}{\partial \theta} \\
& + \quad \frac{\partial}{\partial r} \left(\frac{v_{r(p)} + v_{r(w)}}{2} rh \right) + \frac{\partial}{\partial \theta} \left(\frac{v_{\theta(p)} + v_{\theta(w)}}{2} h \right)
\end{aligned} \tag{5.1}$$

The primary quantity dictating the fluid pressure (p) in the Reynolds Equation (eq. (A.1)) is the film thickness 'h'. The film thickness in this model has been approximated as the separation between the smooth wafer surface, and the mean plane of the pad asperities. The individual contribution of the nominal clearance (δ_0), rolling angle (α) and pitching angle (β) have been superposed to give the effective film thickness at a point (Fig. 5.1). The resultant film thickness can be written as shown in (5.2).

$$h(r, \theta) = \delta_0 + r \sin \alpha \cos \theta + r \sin \beta \sin \theta \tag{5.2}$$

The velocities have been calculated with the wafer's center as the origin, following the work of previous studies by Park et al. [77] Cho et al. [78] and Beschorner and

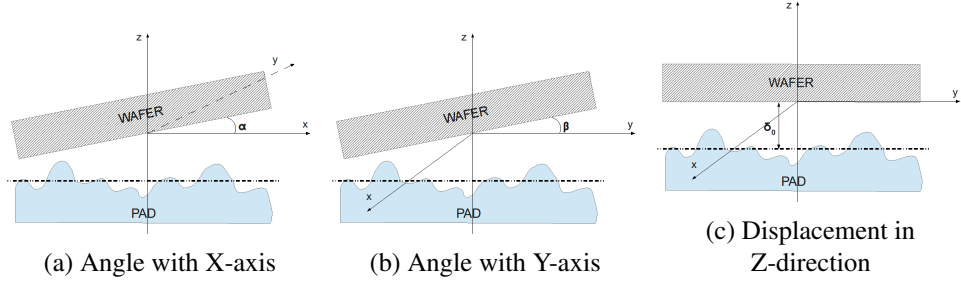


Figure 5.1: Superposition of individual variables to calculate the film thickness

Higgs [66], shown in Fig. 5.2 and can be given as in (5.3)

$$v_{r(p)} = r_{wp} \sin \theta \Omega_p \quad (5.3a)$$

$$v_{\theta(p)} = (r + r_{wp} \cos \theta) \Omega_p \quad (5.3b)$$

$$v_{r(w)} = 0 \quad (5.3c)$$

$$v_{\theta(w)} = r \Omega_w \quad (5.3d)$$

5.2.2 Wafer-Pad Contact

In a regular CMP setup, the pad is made of a soft polymeric material placed on top of a rigid metallic platen. The wafer typically is a metallic, metalloid or ceramic material, and is much tougher than the polymeric pad. Thus, the solid-solid contact between the wafer and the pad can be modeled through a Winkler Elastic Foundation [67] which approximates the softer material as a mattress, constructed by assembling a set of parallel springs. In this case, each spring represents a collection of, or a single asperity, occupying a rectangular area, and representing the average height of that area. It is assumed that these springs deform vertically, without

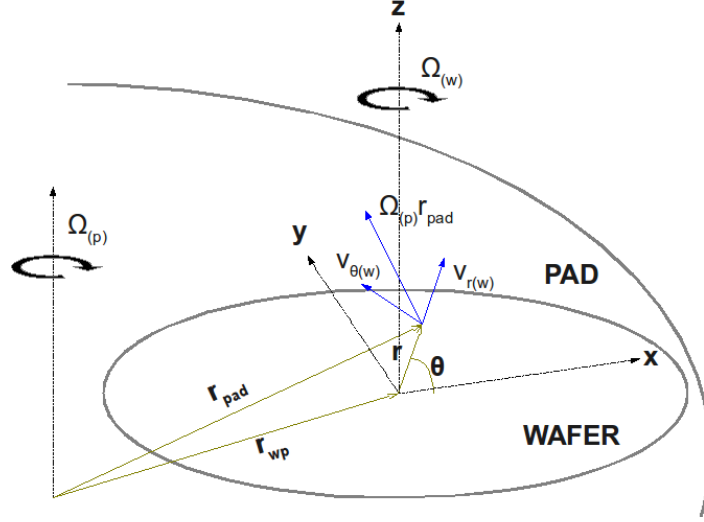


Figure 5.2: Different velocities in the system

influencing their neighbors. This provides a relationship (eq.(5.4)) between the stress and normal deflection for each spring, as has been described by Johnson [67]

$$\sigma(x, y) = K \frac{u(x, y)}{\tau} \quad (5.4)$$

where, σ is the contact pressure, τ is the initial height of the foundation, and u is the deformation at the surface. The following assumptions were made to determine the proportionality constant:

- Tangential deflection of the asperities is neglected
- The effect of the tangential loads on the normal deflection is neglected

With the above assumptions, the equations of elasticity for the pad can be condensed to eq. (5.5)

$$\sigma(x, y) = \frac{E_{pad}(1 - \nu_{pad})}{(1 - 2\nu_{pad})(1 + \nu_{pad})} \frac{u(x, y)}{\tau} \quad (5.5)$$

This expression explicitly relates the normal stress $\sigma(x, y)$ to the normal deflection $u(x, y)$ of an asperity. As a result, the calculation of contact pressure can be obtained through $O(N)$ operations, which is critical to maintaining the speed and memory efficiency of PAML+.

5.2.3 Equilibrium Orientation

The fluid and contact pressure fields are used to formulate three equations in three independent variables mentioned earlier, the nominal clearance (δ_0), rolling angle (α) and pitching angle (β). The three equations correspond to the equilibrium conditions of no normal force ($F_z = 0$), and no tangential moments ($M_x = 0, M_y = 0$) on the wafer. The equations are non-linear, implicit equations and, hence an analytical solution is not possible. A novel root finding method based on a homotopy algorithm has been designed to solve the equations, which is described next.

The algorithm starts with an initial guess, sufficiently far from the expected solution. One of the variables is fixed at the initial value and the remaining two variables are varied to satisfy two of the equations. The first variable is then modified slightly, and the other two variables are again varied to satisfy two equations, starting with the previous iteration's roots as the initial guesses. This process is repeated until the third equation is also satisfied by the values of the three variables.

For the step at solving the two equations, the conjugate gradient method was employed to ensure stability and consistency. As all the equations are non-linear and highly complex, traditional root finding algorithms such as Newton-Raphson, Secant method or Broyden method were found incapable of yielding consistent results.

It is important to note that the equilibrium being discussed here, is a quasi-steady

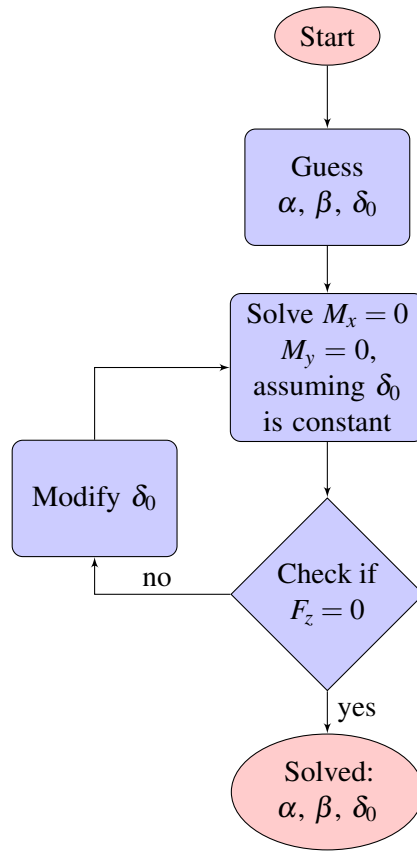


Figure 5.3: Root finding algorithm

equilibrium. As the pad and wafer rotate, the hydrodynamic pressure and the contact stress change and a new equilibrium orientation appears at every time step.

5.2.4 Wear

Abrasive wear has been widely accepted as the predominant wear mechanism during CMP. Following the definition of abrasive wear, a "wafer-wear" event only occurs when an abrasive particle indents into the wafer surface, due to force applied by the pad asperity. The method used for calculating wear over a wafer asperity is based on the formulation described by Luo and Dornfeld [73, 79]. The aggregate plastic

deformation in both wafer and pad (Δ) can be written as:

$$\Delta = \Delta_w + \Delta_p \quad (5.6)$$

where, the subscripts 'w' and 'p' refer to the wafer and the pad respectively. The particle sizes are assumed to follow normal distribution, with the probability distribution function defined as in equations (5.7) and (5.8).

$$p\{d = d_a\} = \frac{1}{\sqrt{2\pi}} \exp \left[-\frac{1}{2} \left(\frac{d - d_{avg}}{\sigma_d} \right)^2 \right] \quad (5.7)$$

$$p\{d \leq d_a\} = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{(d_a - d_{avg})/\sigma_d} e^{-(1/2)t^2} dt \quad (5.8)$$

Every particle having diameter larger than Δ will cause plastic deformation, and hence lead to wear. Following this principle, the number of active particles can be calculated as equation (5.9).

$$\begin{aligned} N_{active} &= N_{total} - N_{d < \Delta} \\ &= N_{total} (p\{d \leq d_{max}\} - p\{d \leq \Delta\}) \end{aligned} \quad (5.9)$$

Here, following the work of ref. [73], it is assumed that the average diameter of the active particles is independent of the down pressure, as in most cases, only the largest particles would be participating in wear. N_{total} is the total number of particles trapped in the interface, which can be calculated through the slurry concentration.

Also, in most cases: $(d_{max} - d_{avg})/\sigma = 3$, and $p\{d \leq d_{max}\} = 1$. The total volume removed at every asperity contact is calculated by adding the volume

removed by every active particle, which in turn is approximated as the product of the number of active particles, and volume removed by one average-sized active particle. Volume removed by one particle is written as equation (5.10).

$$Vol_{avg} = \Delta_w a_w v_{rel} \quad (5.10)$$

where, Δ_w is the particle indentation depth into the wafer surface, a_w is the radius of contact area between the particle and the wafer surface, and v_{rel} is the velocity with which the particle is being dragged across the wafer, which in this case is the relative velocity between the pad and the wafer at that location. Assuming the contact between the particle and the wafer is completely plastic, as shown by ref. [73], Δ_w and a_w can be calculated as (5.11) and (5.12) respectively.

$$\Delta_w = \frac{2F}{\pi d_{avg-a} H_w} \quad (5.11)$$

$$a_w = \sqrt{\frac{2F}{\pi H_w}} \quad (5.12)$$

Using equations (5.11) and (5.12), we can rewrite (5.10) as (5.13).

$$Vol_{avg} = \frac{1}{d_{avg-a}} \left(\frac{2F}{\pi H_w} \right)^{3/2} v_{rel} \quad (5.13)$$

Here, F can be calculated using the contact stress given by equation (5.5), and v_{rel} can be obtained by using equations (5.3). As mentioned earlier, d_{avg-a} is independent of the down-pressure and has been approximated as being close to the size of the largest particles.

Table 5.1: Model Parameters

Pad Properties	
Model Simulated	IC 1000
Elastic Modulus (Bulk)	12 MPa
Elastic Modulus (Tip)	300 MPa
Poisson's Ratio	0.4
Hardness	5.0 MPa
Asperity Distribution	Gaussian
Thickness	1.3 mm
Roughness	5 μm
Wafer Properties	
Elastic Modulus	110 GPa
Poisson's Ratio	0.16
Hardness	2.0 GPa
Slurry Properties	
Solvent	Water
Solvent density	1000 kg/m ³
Abrasives	SiO ₂
Abrasive Density	2000 kg/m ³
Abrasive Size Distribution	Gaussian
Mean Abrasive Diameter	150 nm
Standard Deviation of Abrasive Diameter	70 nm

5.3 Results

The Reynolds Equation was solved numerically using the wafer center as the origin. The entire region under the wafer was discretized into a polar rectangular grid. The pad was independently discretized into another polar grid. For calculating the contact stress, a pad surface was generated with a mean height and average roughness specified in Table A.1.

Figure 5.3 shows the overall algorithm that was followed in the model for the transient analysis. As shown, the equilibrium hydrodynamic pressure and contact stress profiles are calculated at every time step, as is the wafer wear. Note that the

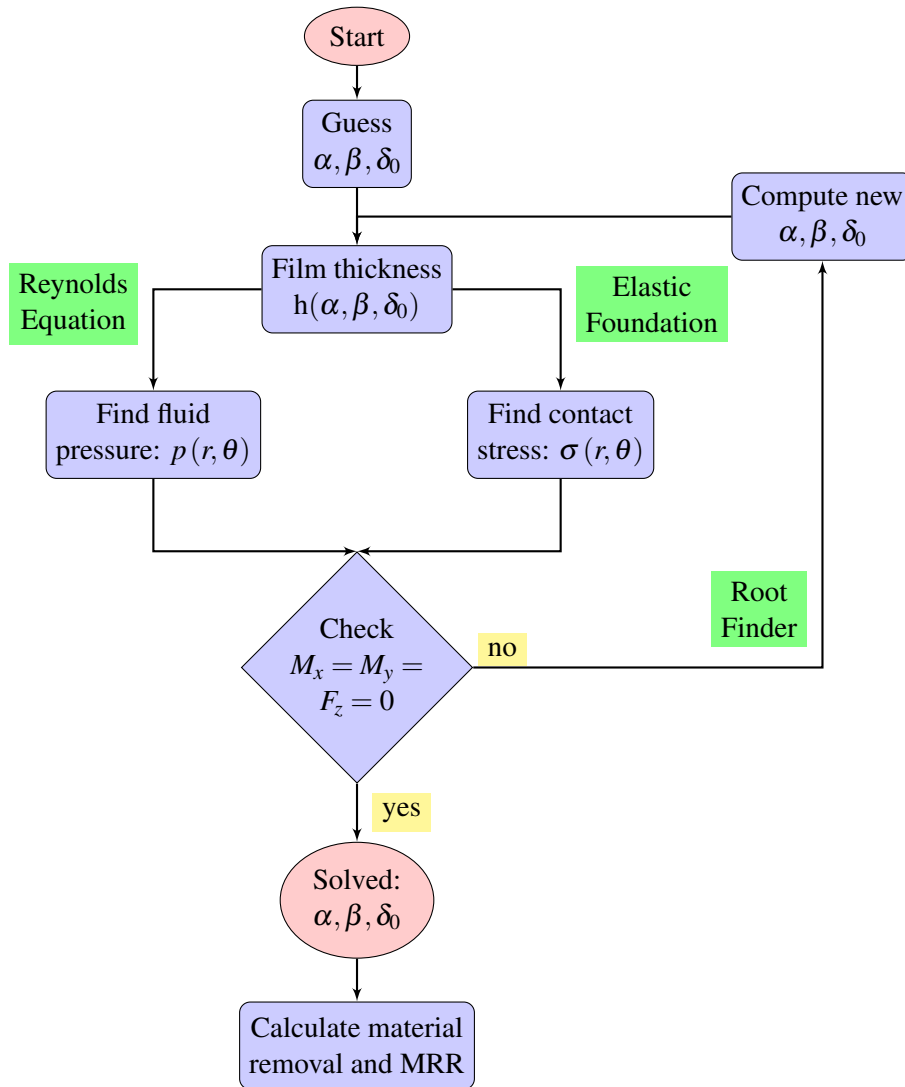


Figure 5.4: Flowchart of the modeling process

model provides a wear "field" as an output, which is then averaged over the entire region for comparing with other studies, which typically give an average material removal rate in terms of reduction in thickness of the wafer.

5.3.1 Fluid Pressure

The model can predict the evolution of the hydrodynamic pressure profile over the course of a simulation. Over the entire simulation, no steady state pressure profile is observed. This is not surprising as the surface of the pad affects the equilibrium orientation, which in turn governs the distribution of fluid pressure. As the surface of the pad is rough with significantly different topographies interacting with the wafer in consecutive time steps, a new equilibrium orientation and thus a new pressure profile is expected at every time step. However, an "average fluid pressure field" can still be calculated by averaging the pressure field over one whole rotation of the pad. This average pressure was compared against the measured fluid pressure reported by Osorno [80] for conditioned pads in Fig. 5.5. The experimental measurements were conducted through wireless point probes that rotated with the wafer. These discrete values reported by the point probes were then interpolated to construct a pressure contour. Ignoring the zig-zag nature of the pressure distribution which appears to be the artifact of the spatial interpolation, good agreement can be observed between the model and the experiments.

5.3.2 Polishing Load

The effect of the polishing load on the material removal rate was compared against the numerical and experimental calculation of Terrell and Higgs [61], as shown in Fig. 5.6. It can be seen that for lower loads (less than 16 psi) the model is in good

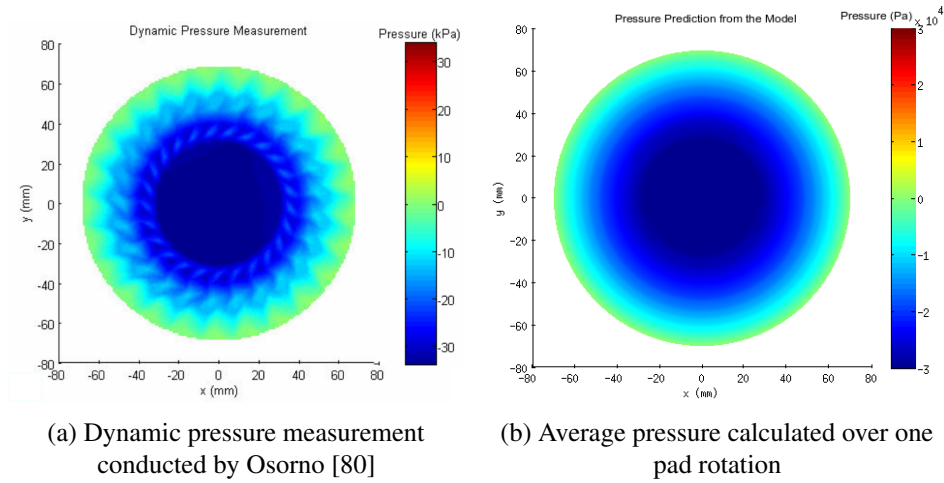


Figure 5.5: Dynamic fluid pressure profile for a well conditioned pad

agreement with the experimental measurements and is closer than the numerical results generated by the PAML model [61]. However for higher loads, the deviation between the experimental results and the current model becomes much greater, which can be attributed to the approach taken to model the contact mechanics in this work. As discussed in 5.2.2, the pad has been modeled to act as an assembly of independent voxels that do not influence each other while deforming under stress. As the springs (and hence the representative voxels) act independently, they only come in contact when the applied load is large enough to cause deformation in all the asperities taller than themselves. Because of this, as the load increases, patches of pad start to appear that have been deformed completely flat, i.e. no difference in the heights of the deformed voxels. This leads to the fluid getting incrementally squeezed out of the interface. This in turn results in unrealistically large loads being supported through the solid-solid contact between the wafer and the pad. Such high contact stresses would lead to much higher material removal as is seen in the

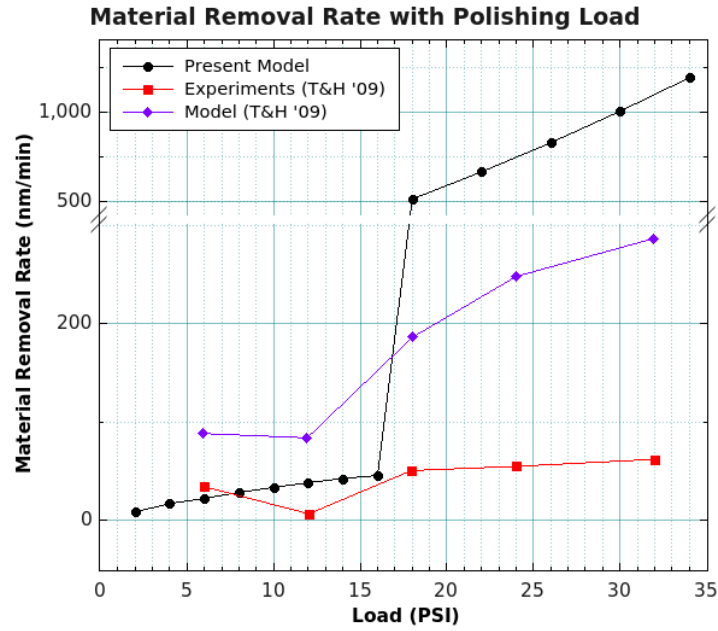


Figure 5.6: Effect of polishing load on the material removal rate

Fig. 5.6. Fortunately, more and more applications now seek very low after-polish roughness values. The general strategy to achieve such low roughnesses is to apply very low loads during polishing. In such cases, the present model can provide excellent predictions.

5.3.3 Particle Size and Concentration

The effect of the abrasive particles in the slurry was also studied in this section. The material removal rate predictions of the model have been compared against the experimental data reported by Biemann et al. [81] who studied the effect of different particle sizes and solid concentration on the MRR. Figure 5.7 plots the variation in the MRR as a function of solids loading. For the lower concentrations (less than 15%), the linear increase in the MRR with increasing the solid concentration

matches well with the experimental observation by Biemann et al. (shown in the inset). However, two major differences can be noted between the two set of results.

Firstly, in the experimental data, one can observe the saturation of MRR for smaller particles above the concentration of 10%. It has been explained in detail by [82] that at higher concentrations, the MRR saturates and does not increase with increasing the solid loading. After the saturation point, in the absence of exposed wafer surface, additional adhesives cannot come in contact with the wafer and hence fail to cause any additional wear. Thus, a larger fraction of available abrasives remains "*inactive*", and possibly enhances lubrication, similar to lubrication enhancement caused by granular media [83,84]. As the current model fails to account for the inactivity in a larger fraction of particles beyond a certain point, similar phenomena is not reflected in the results of the present model.

Secondly, although the variation in MRR in the experimental data is linear (Fig. 5.7 (inset)), there appears to be a non-zero y-intercept to all the curves plotted. On the other hand, the present model shows that all the curves pass through the origin, thus resulting in zero intercept. This difference can be explained by the assumption made for the present model which ignores all wear mechanisms except abrasive wear. This means that there would be no wear predicted by the model when the solid concentration goes to zero, i.e. in an abrasive free slurry. During the experiments, however, some material removal may still be possible in the absence of particles as a result of chemical erosion which has been neglected in this study.

The dependence of MRR on mean abrasive particle diameter has also been studied. As noted by Biemann et al. [81] and followed on by [79], the material removal rate drops exponentially with increase in the abrasive particle diameter. Similar behavior has been observed in the present study as shown in fig. 5.8a. The

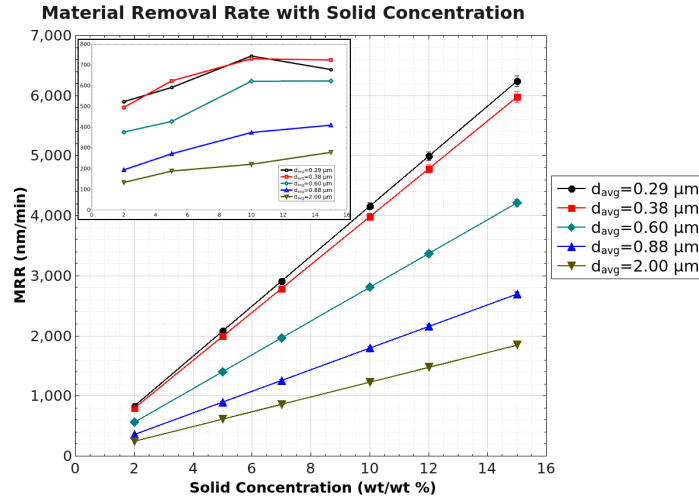


Figure 5.7: Material removal rate with varying abrasive concentration in the slurry, plotted for various mean abrasive diameters. *Inset*: Data presented by Biemann

MRR averaged over concentration values in the linear region in fig. 5.7 (2%, 5% and 10%) has been plotted against mean abrasive particle diameter.

Although trend-wise similarity has been observed in both these comparisons, quantitatively, the values reported by the present study have been off by a factor of 3 to 4. This can be explained by the uncertainty in the values of the input parameters required for the model. For this comparison, most common values have been used for the material properties of the wafer and the pad and operating parameters were estimated from the limited information available in Biemann et al.'s paper [81]. If the model predictions are multiplied by a constant scaling factor to account for all these uncertainties, an excellent match can be obtained between the predicted values and the experimental measurements, as shown in fig. 5.8b. Similar approach has been followed by [79] while comparing their modeling approach against the experimental data reported by [81].

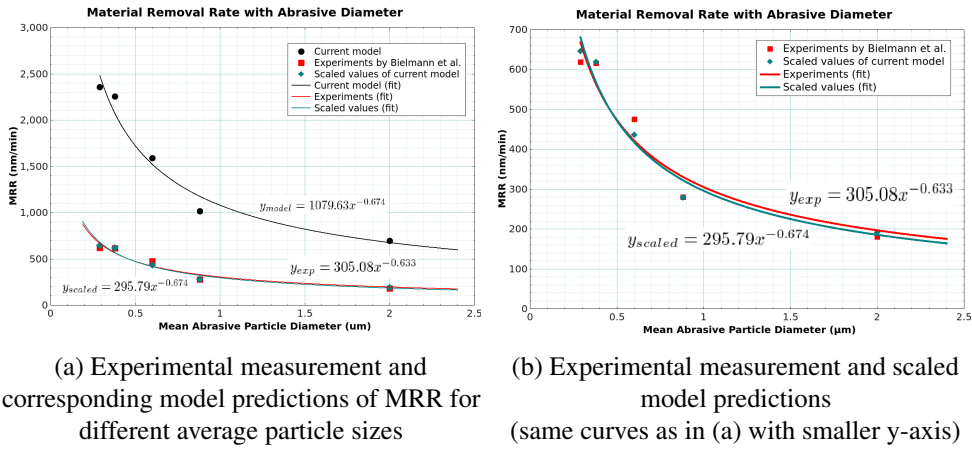


Figure 5.8: Material removal rate as a function of average particle size

5.3.4 Parametric Studies

Now that different aspects of the model have been validated against experimental measurements, parametric studies were conducted to understand the effect of parameters that are difficult to study experimentally.

Slurry Viscosity

Several researchers have reported several degrees of temperature increase during polishing [85–87]. Thus, the performance of the slurry can differ significantly with such changes in temperature. One of the most prominent effects of the increase in temperature can be seen by a sharp decrease in the slurry viscosity. Through the present model, the effect of such change in viscosity has been studied and the result is shown in Fig. 5.9. It can be seen that material removal rate decreases rapidly with increases in viscosity. This is expected, as with increase in viscosity the load carrying capacity of the fluid increases, resulting in reduced solid-solid contact stress between the wafer and the pad. The increase in the load carrying

capacity can also be monitored by the fluid pressure in the interface. Figure 5.10 shows the time averaged fluid pressure distribution in the interface for three of the studied viscosity values (the Z-axis limits have been adjusted for each plot to show the pressure profile). Even though the pressure profile remains similar, a steady increase in the pressure values can be observed as the viscosity increases. The sharp increase in the pressure can be even clearly noted through Fig. 5.11 which plots the same data for common Z-axis limits.

In absence of any solid-solid contact, as might be the case with the slurry viscosity equal to 0.01, there would be virtually no material removal (once again, here we are assuming that particle abrasion is the only mechanism for wafer wear and effects of erosive material removal have been neglected). As the temperature rises with time during the polish, thus resulting in lower viscosities, one can expect faster material removal than at initial, ambient temperatures.

Particle Size Distribution

Controlling the abrasive particle shape and size is a very difficult task due to the inherent nature of the process by which they are produced. Also, it is extremely difficult to study the effect of degree of deviation from the mean abrasive size experimentally, as the deviation itself is not a controlled parameter but a result of inefficient manufacturing. This is where computational tools like the present model can provide invaluable insight. Assuming all the particles are spherical, the effect of deviation from the mean value of the particle diameter was studied. Figure 5.12 shows the variation in material removal rate with change in the standard deviation of the diameter of the particles. One expects the change in standard deviation to not cause much variation in MRR, since with increasing the standard deviation,

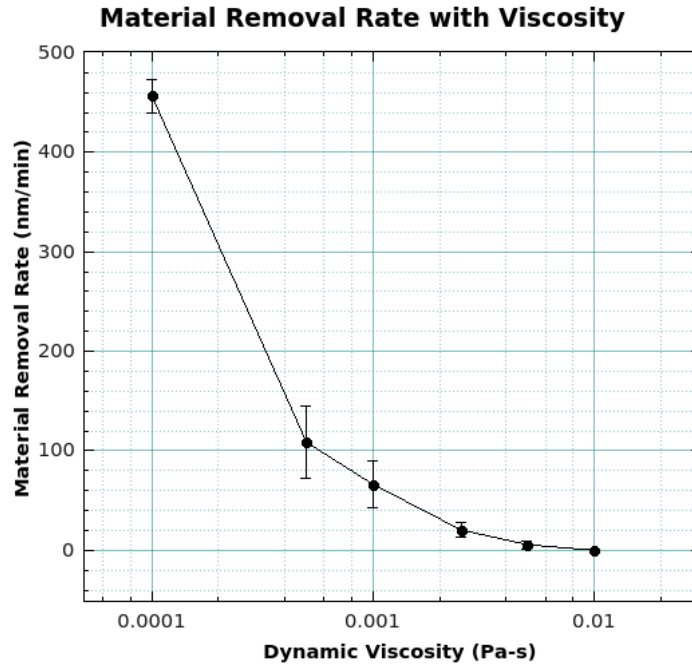
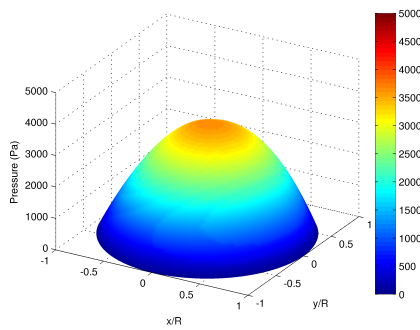
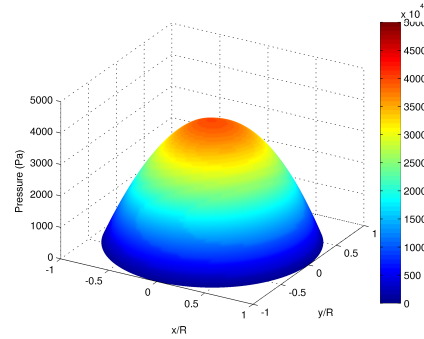


Figure 5.9: Effect of newtonian slurry viscosity on the material removal rate

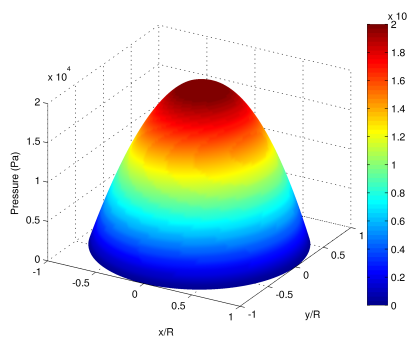
two counteracting effects come into picture. Firstly, for a particle size distribution with large standard deviation, the active particles would have larger diameter, than the distribution with smaller standard deviation. As seen in section (5.3.3), larger particle sizes would be expected to cause lesser material removal. On the other hand, having a larger standard deviation would lead to a larger fraction of particles being active particles. To understand this, consider the scenario where the standard deviation is very small i.e. all the particles are of roughly the same size. One can imagine that in such a case, all the particles would be contacting the wafer and the pad in a similar manner. As a result, the load from the pad would be distributed evenly among all the particles leading to each particle getting a small fraction of the contact load. Depending on the pad asperity pressure, such small loads would be



(a) Viscosity = 0.0005 Pa-s



(b) Viscosity = 0.001 Pa-s

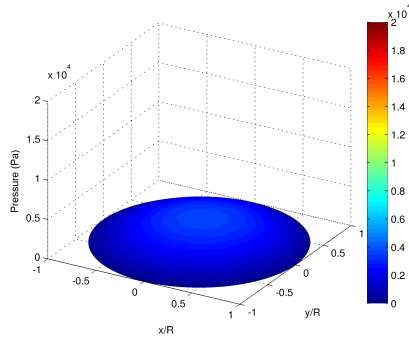


(c) Viscosity = 0.005 Pa-s

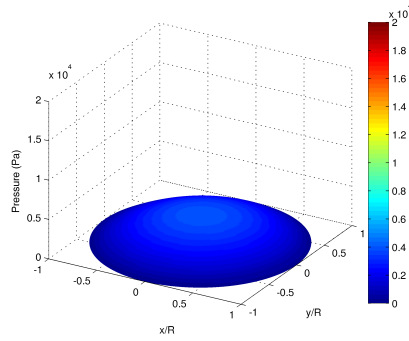
Figure 5.10: Average fluid pressure as a function of viscosity (locally scaled Z axis)

more likely to cause elastic deformation in the wafer surface and hence would result in a larger fraction of inactive particles. Thus, having larger standard deviation should lead to more active particles, and hence more wear.

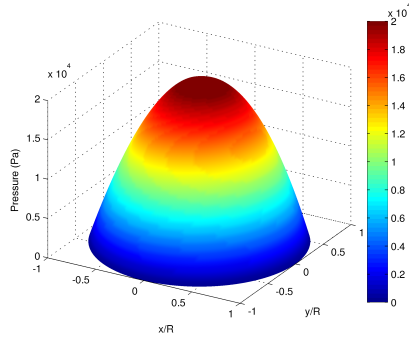
As seen in fig. 5.12 a larger variation in particle sizes, indicated by a larger standard deviation of particle diameter results in slightly higher average material removal rate. This suggests that having more active particles has a stronger effect than having lower material removal per particle. However, the wafer polished with a slurry having a larger variation in particle sizes would have a higher probability of resulting with polishing defects such as micro-scratching and pitting [88]. On the



(a) Viscosity = 0.0005 Pa-s



(b) Viscosity = 0.001 Pa-s



(c) Viscosity = 0.005 Pa-s

Figure 5.11: Average fluid pressure as a function of viscosity (universally scaled Z axis)

other hand even though we would get much more control on the surface quality with a very small variation in particle sizes, the cost of such control might be prohibitive, and would also result in a much slower polish. Thus, aiming for a median standard deviation value in particle sizes would be easier to achieve and would also yield an acceptable surface quality.

5.3.5 Model Limitations

The presented model has several limitations. Firstly, the model overpredicts the material removal in the cases of higher loads. This can be attributed to the simplified

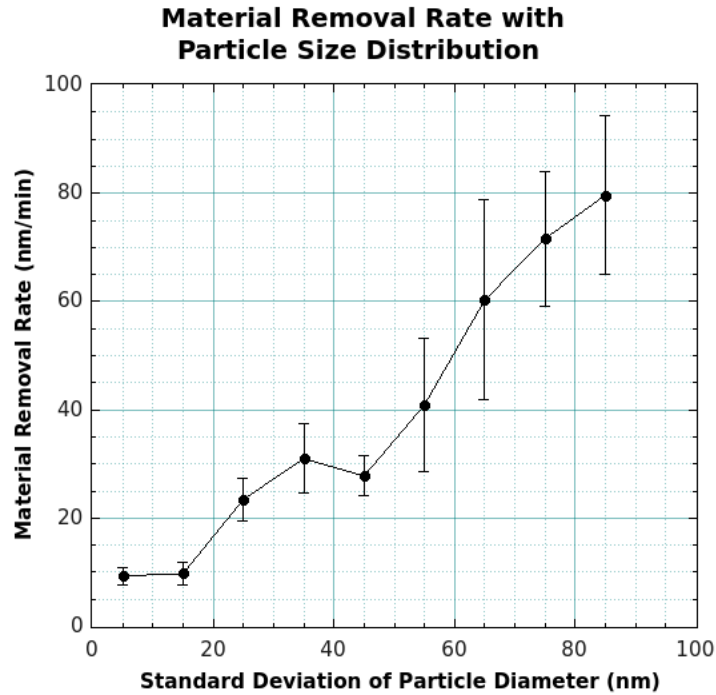


Figure 5.12: Effect of particle size distribution on the material removal rate, for a mean particle size of 150 nm

contact mechanics formulation, leading to the model's inability to capture the influence of one asperity deflection on the its neighboring asperities. The lack of this interaction leads the model to predict “dry” conditions before they occur in reality, thus predicting higher material removal rates. Another limitation for the model is the lack of chemical interactions, the effects of which can be clearly seen in the particle size comparison study 5.3.3. As seen in Fig. 5.8a, the model overpredicts the material removal rate for all particle diameters. However, the model matches excellently with the experimental data once the values are scaled by a constant factor. This scaling factor has been used by several researchers as an empirical coefficient representing the chemical effects. Thus, a phenomenological

model of the chemical interactions would bring the model predictions closer to reality. Until then, the current model would not be suitable to simulate the scenarios dominated by chemical interactions.

5.4 Conclusion

A new multiphysics model based on the hypothesis of abrasive wear and particle augmented mixed lubrication was developed for wafer-scale analysis of CMP. The model integrated the effects of mixed lubrication in the wafer-pad-slurry interface, and wear caused by the abrasive particles in the slurry. The hydrodynamic pressure field was solved using the Reynolds lubrication equation for cylindrical polar contacts. The average fluid pressure profile thus calculated at the equilibrium orientation agrees well with previous experimental measurements. An elastic foundation model was implemented to evaluate the stress field for the rough contact between the elastic polymeric pad and rigid silicon wafer. The equilibrium configuration for the wafer was determined by solving three simultaneous non-linear integral equations generated using the pressure and contact stress fields. Material removal is calculated assuming abrasive wear action caused by hard slurry particles getting trapped between the asperity contacts. A variety of temporal and time-averaged quantities can be obtained as the output of the model. The average fluid pressure distribution obtained from the model matches well with the experiments conducted by [80]. The effect of variation in polishing load on the material removal rate also agrees with the experiments conducted by the authors in the past [61]. Finally, the effect of abrasive particle diameter and solid loading of the slurry also matches with papers published in the past [79, 81].

The model can capture wafer-scale defects such as differential polishing across the wafer and over-polishing close to the wafer edge. With the model's capability to capture multiphysical interactions, the effect of several material or operational parameters can be studied. The model can thus provide invaluable insights in the cases where the parameter of interest can be prohibitively expensive or outright impossible to study experimentally. This capability was demonstrated through two example cases of variation in slurry viscosity and abrasive particle size distribution. Such a powerful model can facilitate design and evaluation of the next generation of polishing equipment and consumables, thus reducing the cost of electronic devices.

Chapter 6

Applications: Artificial Hip Joints Model

Note: The model described in this chapter has been filed as an intellectual property by Carnegie Mellon University (CMU). Any for-profit use of the modeling approach described herein requires contacting the CMU Center for Technology Transfer and Enterprise Creation (CTTEC)

6.1 Introduction

Total hip replacements have extended the mobility of athletic and sedentary patients for nearly half a century. The introduction of total hip replacements in the mid 1960s particularly by McKee and Watson-Farrar [89] and Charnley [90] started the modern era of successful joint replacements. Where the former introduced the metal-on-metal 'bearing', the latter used the metal-ball-on-polyethylene socket arrangement, which

was vastly succesful clinically. This led to introduction of metal-on-polymer type of replacement joints for other body parts such as the shoulder, knee, ankle, elbow and recently, spinal discs.

Although the hip and knee replacement has been hugely popular among the surgical community, degradation of the artificial joints has been a matter of concern for the bio-mechanical engineers and clinicians. Ultrahigh molecular weight polyethylene (UHMWPE) wear particles generated at the articulating surface of acetabular cup are strongly linked to osteolysis about those implants [91] [92] [93]. Several studies have demonstrated the presence of polyethylene debris in osteolytic tissue from hip [91] [94] [95], knee, [96] [97] [98] and shoulder [99] arthroplasties. Several authors have suggested it is reasonable to assume that polyethylene particles alone can lead to osteolysis, because osteolysis occurs in the absence of identifiable metallic or polymethylmethacrylate particles [95]. Unfortunately, these particles are not just a local problem close to the prosthesis. Urban et al. [100] studied the dissemination of debris particles in patients with total hip and knee replacements by looking at tissue from the liver, spleen, and lymph nodes. Polyethylene particles were identified in the para-aortic lymph nodes of two-thirds of those patients and in the liver or spleen of about a seventh of them. The mechanism of biological response to UHMWPE particles has been understood to be a very complicated process. However there is consensus among the researchers that particle size, morphology, and concentration play a significant role in this response [101] [102].

The adverse tribological conditions in the hip joint interface, such as low speeds and fluid viscosities, in addition to high impact loads, cause the lubrication mode to exist in the boundary and mixed lubrication regimes [103] [104] [63]. These regimes drastically reduce joint lifetimes since they can lead to increased wear debris

generation and the onset of osteolysis. The tendency of failure via the generation of wear debris has turned the hip problem into a serious bio-tribological challenge. Therefore, researchers have worked to develop hip joint interfaces which are robust against wear and debris generation.

In tribology, surface texturing in the form of micro-cavities has been shown to provide enhanced wear resistance in two ways. First, abrasive wear debris can be trapped in the micro-cavity reservoirs [105] [106]. Second, enhanced fluid pressures which promote better lubrication at low speeds have been generally reported in textured sliding contacts [107] [108] [109] [110]. Therefore, it is the objective of this investigation to simulate the effect of surface texturing in metal-on-UHMWPE total hip replacements using a particle augmented mixed lubrication (PAML) computational modeling framework. In PAML, the tribological behavior of the hip joint interface under walking conditions is simulated using integrated lubrication, contact mechanics, particle mechanics, and wear modeling. Real surface femoral head and acetabular cup topographies and properties are considered, along with the evolution of the fluid pressure, contact stress, and wear for various textured hip joint cases.

6.2 Modeling

A computational model, based on the principles of mixed lubrication and adhesive/abrasive wear has been constructed to study the influence of surface topography and texturing on the life-time of artificial hip joints. The mixed-lubrication modeling approach is based on the premise that the artificial hip-joint operates in a quasi-steady state, instantaneous equilibrium. This state of quasi-equilibrium is

achieved when the net forces acting on the femoral head, vanish. The major loads acting on the femoral head - acetabular cup interface during normal walking gait are the hydrodynamic pressure applied by the slurry, the contact stress between the femoral head and acetabular cup asperities and the patient's body weight. The following assumptions have been made to make the analysis simpler:

- The flow of the synovial fluid in the interface is assumed to be incompressible and Newtonian (although some authors have shown the synovial fluid to be a shear thinning fluid, that behavior is observed at very high shear rates, which are not common during normal operation)
- The acetabular cup lining material (UHMWPE) is assumed to be linear-elastic and isotropic
- The textures are assumed to be uniform across the surface of the femoral head

Based on the assumptions listed above, a comprehensive model is presented here that accounts for the effect of the synovial fluid, solid - solid contact between the acetabular cup and the femoral head, and wear due to sliding between the two solids. Figure 6.1 summarizes the major components of the model. The following sections describe those steps in detail.

6.2.1 Synovial Fluid

The effect of synovial fluid on the operation of an artificial hip joint has been widely acknowledged in several studies. Many authors have even assumed the operation of the hip-joint to be in an elasto-hydrodynamic lubrication regime, thus basing their model on calculation of the fluid pressure [111] [111] [112] [51] [113].

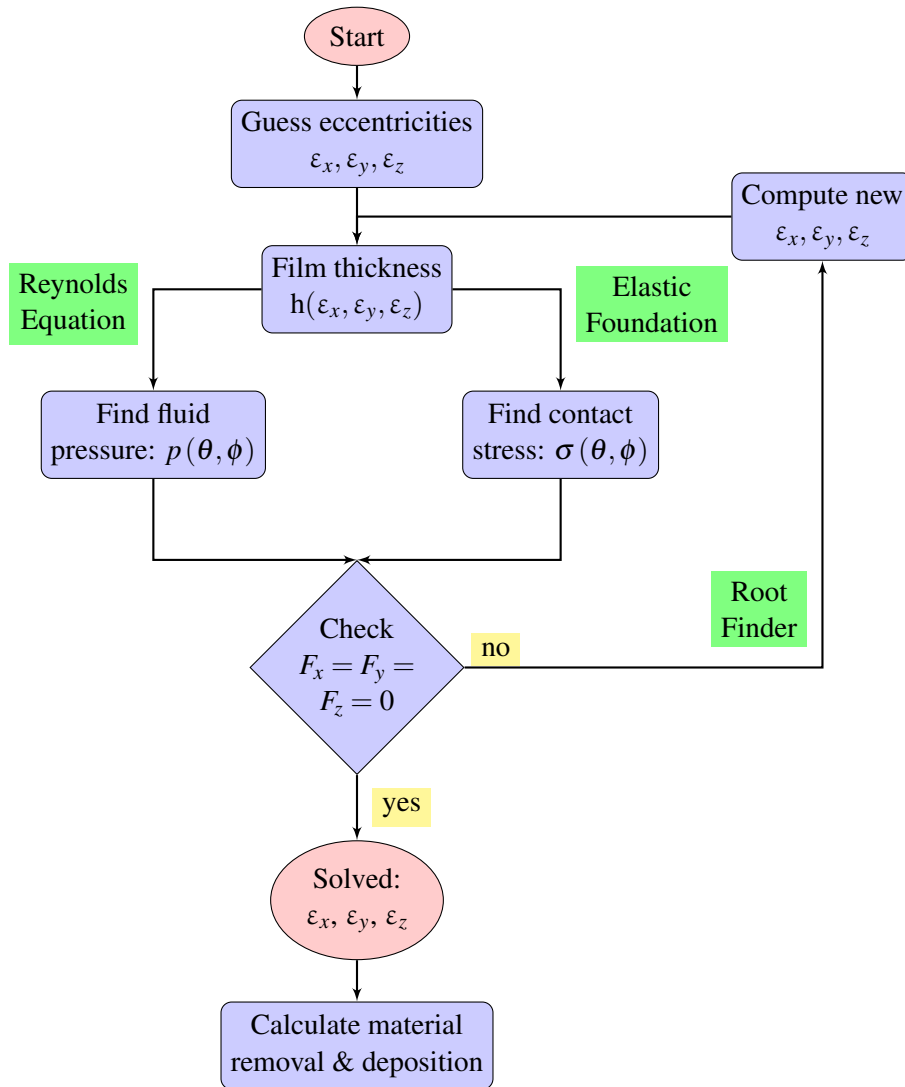


Figure 6.1: Flowchart of the modeling process

The present model also integrates the effect of the synovial fluid as an important part of the analysis, and includes the hydrodynamic pressure to determine the equilibrium configuration of the femoral head. Similar to the authors previously mentioned, the spherical Reynolds equation (6.1) has been used to calculate the generated hydrodynamic pressure between the two surfaces. The most general form of the Reynolds equation [114] is being solved to model the more realistic, three dimensional articulation of the hip-joint.

$$\begin{aligned} \frac{1}{6\mu R^2 \sin \theta} \left[\sin \theta \frac{\partial}{\partial \theta} \left(h^3 \sin \theta \frac{\partial p}{\partial r} \right) + \frac{\partial}{\partial \phi} \left(h^3 \frac{\partial p}{\partial \phi} \right) \right] = \\ 2 \frac{\partial h}{\partial t} + (-\omega_x \sin \phi + \omega_y \cos \phi) \sin \theta \frac{\partial h}{\partial \theta} + \\ (-\omega_x \cos \phi \cos \theta - \omega_y \sin \phi \cos \theta + \omega_z \sin \theta) \frac{\partial h}{\partial \phi} \end{aligned} \quad (6.1)$$

The primary quantity dictating the pressure field in the Reynolds equation is the film thickness 'h'. The film thickness in this model has been approximated as the separation between the smooth femoral head surface, and the mean plane of the acetabular cup asperities. The film thickness is thus calculated based on the eccentricity of the center of femoral head with respect to the center of the acetabular cup, as given in equation (6.2). For the simplicity in presentation here, the motion of the femoral head is assumed to be in the form of three dimensional harmonic oscillation about the center. However, any complex motion profile of the femoral head can easily be handled by the model.

$$h(\theta, \phi) = c(1 - \varepsilon_x \sin \theta \cos \phi - \varepsilon_y \sin \theta \sin \phi - \varepsilon_z \cos \theta) \quad (6.2)$$

6.2.2 Acetabular Cup - Femoral Head Contact

In an artificial hip joint, the acetabular cup is built by placing a compliant polymeric (UHMWPE) liner within a rigid metallic backing. The femoral head typically is a metallic, metalloid or ceramic material, much tougher than the polymeric cup liner. The solid-solid contact between the acetabular cup and the femoral head can hence be modeled through a Winkler Elastic Foundation [67] which approximates the softer material as a mattress, constructed by assembling a set of parallel, bounded springs. In this case, the asperities on the acetabular cup were modeled as independent springs occupying a spherical shell constructed by the polymeric liner. This gave us the following relationship between the stress and the deflection, as has been described by Johnson [67]

$$\sigma(\theta, \phi) = K \frac{u(\theta, \phi)}{h} \quad (6.3)$$

where, p is the contact pressure, h is the initial height of the foundation, and u is the deformation at the surface. The following assumptions were made to determine the proportionality constant:

- Tangential deflection of the asperities is neglected
- The effect of the tangential loads on the normal deflection is neglected

With the above assumptions, the equations of elasticity for the pad can be condensed to equation (6.4)

$$\sigma(\theta, \phi) = \frac{E(1-\nu)}{(1-2\nu)(1+\nu)} \frac{u(\theta, \phi)}{h(\theta, \phi)} \quad (6.4)$$

The following assumptions were made to determine the proportionality constant: This expression explicitly relates the normal stress (σ) to the normal deflection (u) of an asperity. As a result, the calculation of contact pressure can be obtained through $O(N)$ operations, which is critical to maintaining the speed and memory efficiency of the model.

6.2.3 Equilibrium Orientation

The hydrodynamic pressure field and the contact stress field are used to formulate three equations in three independent variables mentioned earlier, namely the eccentricities in the three dimensions. The three equations correspond to the equilibrium conditions of no net force on the interface, eq (6.5) and their solution gives us the quasi-equilibrium orientation. Because the equations are non-linear and implicit, their analytical solution is not possible. A novel root finding method (fig 6.2) based on the homotopy algorithm has been designed to solve the equations, which is described next.

$$F_x = W_x - \int_0^\pi \int_0^\pi (p + \sigma) \sin \theta \cos \phi \sin \theta d\theta d\phi \quad (6.5a)$$

$$F_y = W_y - \int_0^\pi \int_0^\pi (p + \sigma) \sin \theta \sin \phi \sin \theta d\theta d\phi \quad (6.5b)$$

$$F_z = W_z - \int_0^\pi \int_0^\pi (p + \sigma) \cos \theta \sin \theta d\theta d\phi \quad (6.5c)$$

The algorithm starts with an initial guess for the roots, which is sufficiently far from the expected solution. Then one of the variables is fixed at the initial value and the remaining two variables are varied to satisfy any of the two equations. If the third equation is not automatically satisfied, the first variable is then modified

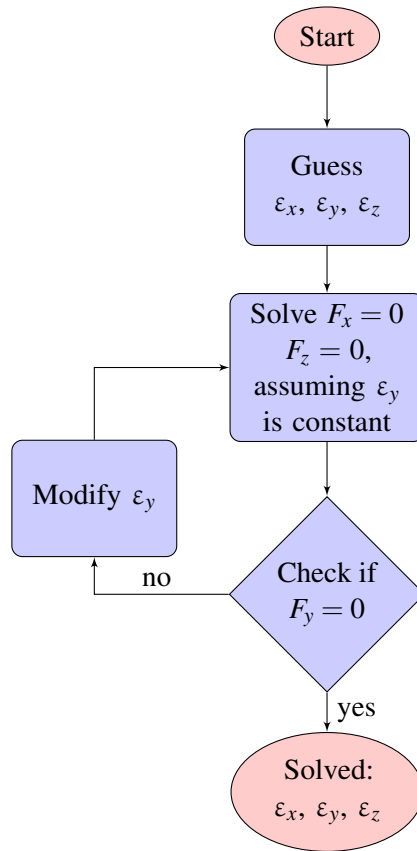


Figure 6.2: Root finding algorithm

slightly. The other two variables are again varied to satisfy the two equations, with the previous iteration's roots as the initial guesses. This process is repeated until the third equation is also satisfied by the values of all the three variables. It was found that traditional root finding algorithms such as Newton-Raphson, Secant method or Broyden method were unsuccessful in solving the equations. So, at the step for solving the two equations $F_x = 0$ and $F_z = 0$, a conjugate gradient based algorithm was employed to ensure stability and consistency. It has been emphasized that the equilibrium being discussed here, is a quasi-steady equilibrium. With time,

as the femoral head moves, the hydrodynamic pressure and the contact stress would change and a new equilibrium orientation will appear.

6.2.4 Debris Generation

Adhesive wear formulation given by Archard [6] in the form of his wear law (eq. (6.6)) has been used. At every asperity contact, the wear law is applied and thus a wear distribution over the entire acetabular cup surface can be constructed. Figure 6.15b shows one such wear map of the acetabular cup.

$$Volume = K_{wear} \frac{F * V_{rel}}{H_{cup}} \quad (6.6)$$

The debris thus generated after the wear action is then distributed in particles of a constant average size. Several studies have reported that the debris generated in the artificial hip joint is typically between the size of 0.01 - 5 μm [115] [91] [93]. To stay well within the general size range, the average size of the debris particle was chosen as 0.1 μm . It is assumed that the generated debris particles transport themselves fast enough, that in the time scales considered, concentration of the debris particles remains uniform in the entire volume of the synovial fluid. This assumption becomes increasingly valid as time progresses and overall concentration of debris increases.

The debris particles while being transported, will settle down on the surface of the femoral head, provided there is an attractive potential between the materials. To calculate the fraction of debris depositing, the migration algorithm given by Yew et. al [116] has been implemented. Although their algorithm was constructed for transportation of nutrients, it is still applicable here for the following reasons.

Firstly, the density of the debris particles is pretty close to that of the synovial fluid. It is not explicitly mentioned in their algorithm but it can be safely assumed that as the nutrients being transported are biological molecules, their density should not be much different from that of water. Hence the inertial effects in the current model are similar to those in effect in Yew et. al's [116] analysis. Moreover, due to their small size and Brownian motion being the governing mechanism for diffusion, the diffusion coefficient for the debris particles is also pretty close to the diffusion coefficient assumed by Yew et. al [116]. Thus, with both inertial and diffusive interactions being similar, we can expect the transportation of debris particles to be tackled by the same algorithm. This diffusion of the debris particles to eventually settle on the surface of the femoral head is going to be a relatively 'slow' process, as was shown by Yew et. al [116]. But in the time scales being modeled here, it can safely be assumed that the diffusion achieves a steady state within one time step.

The volume of deposited particles is estimated by calculating the volume of the fluid having Peclet number lesser than a threshold value. Peclet number, as shown in eq (6.7) is defined as the ratio of the advective and diffusive transport in the suspension.

$$\frac{\text{Advection}}{\text{Diffusion}} = Pe = \frac{d \cdot u}{D} \quad (6.7)$$

$$\text{here, } D = \frac{kT}{3\pi\mu d}$$

where, D is the diffusion coefficient, k is the Boltzmann constant, T is the absolute temperature, μ is the viscosity of the fluid, u is the velocity and d is the diameter of the particle.

It is assumed that the synovial fluid acts as a colloidal suspension and hence the

diffusion of the particles is due to their Brownian motion. When the Peclet number is lesser than the threshold value (assumed to be 0.1 here, following Yew et al. [116]), diffusion is the dominant mechanism for particle transportation. Assuming the bottom surface of the texture is designed to act as a 'sink' for debris, the particles will migrate from higher concentration (near the cup) to lower concentration (bottom of the texture), thus trapping the debris particles from re-entering the circulation.

6.3 Results and Discussion

6.3.1 Hip Motion and Loading

The hip joint undergoes complex three dimensional articulation. As mentioned in the previous sections, the artificial hip joint operates in a manner similar to a natural hip joint. It undergoes three dimensional angular motion, while being loaded under a three dimensional load. Figure 6.3 shows the three motions: flexion-extension (F-E), abduction-adduction (A-A), and internal-external rotation (I-ER), independently, with reference to the anatomical coordinate axes.

While in motion, the hip joint has three degrees of freedom (e_x, e_y, e_z) , that allow translation in three directions to obtain dynamic equilibrium. Several authors have attempted to quantify the motion and loading of artificial joints. Brand et al. [6] and Bergmann et al. [7] in their seminal works, quantified the motion and loads experienced by a variety of patients during walking. However, most of the *in situ* information about the operation of an artificial joint is obtained through hip simulators that try to replicate the motion of a natural joint thorough an approximate, preset load and motion conditions. There have been several of papers from the inventors of a variety of hip joint simulators. The load and motion conditions

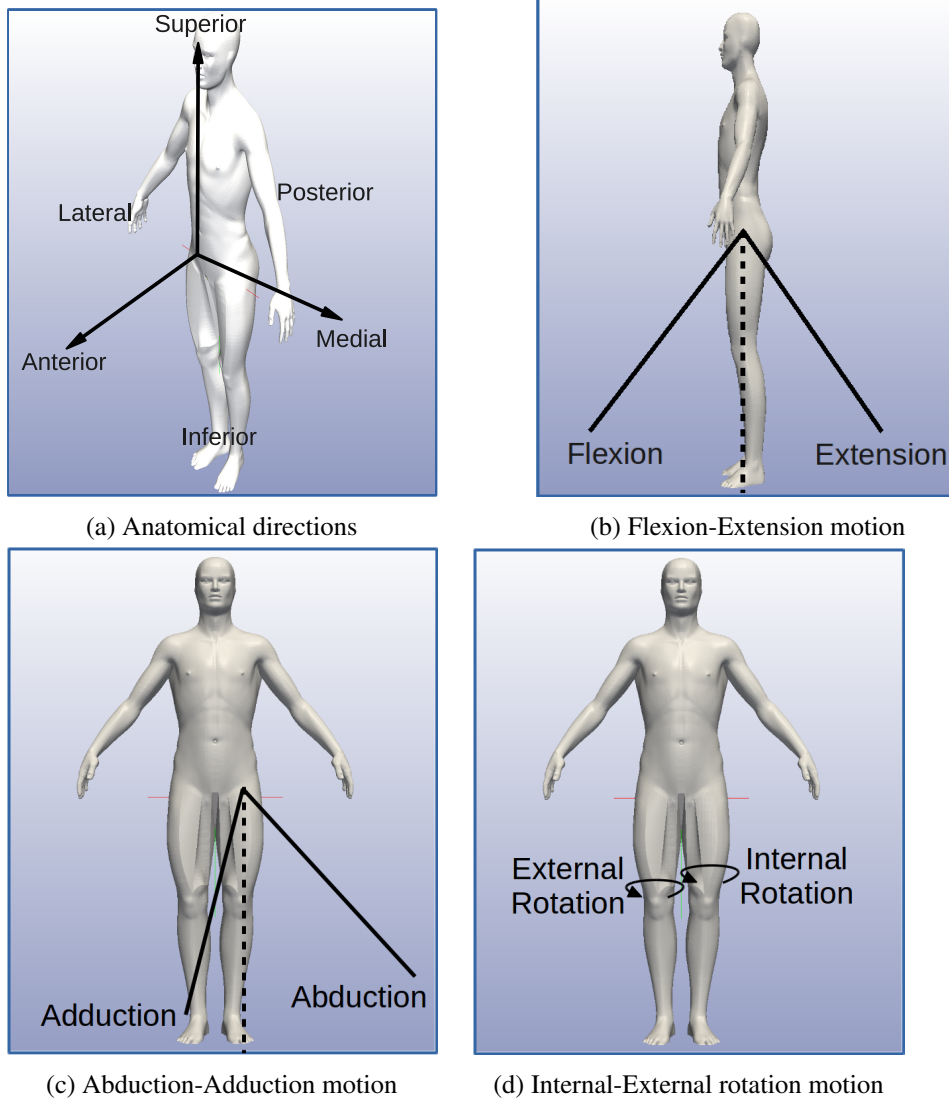


Figure 6.3: Three motions of the hip joint

generated by the single-station electromechanical-pneumatic apparatus, known as HUT-3 have been used in this work, unless otherwise stated. The operation and simulated load and motion conditions have been described in detail by the inventor Vesa Saikko in their paper [6]. The following sections discuss the motion and load

conditions briefly, and outline the process followed to incorporate a general loading condition in to the model.

Step 1: Input

The paper by Saikko presents their motion and load graphically, through an image (fig. 6.4) generated from an oscilloscope, which represents the waveforms of the three dimensional displacements and loads over time.

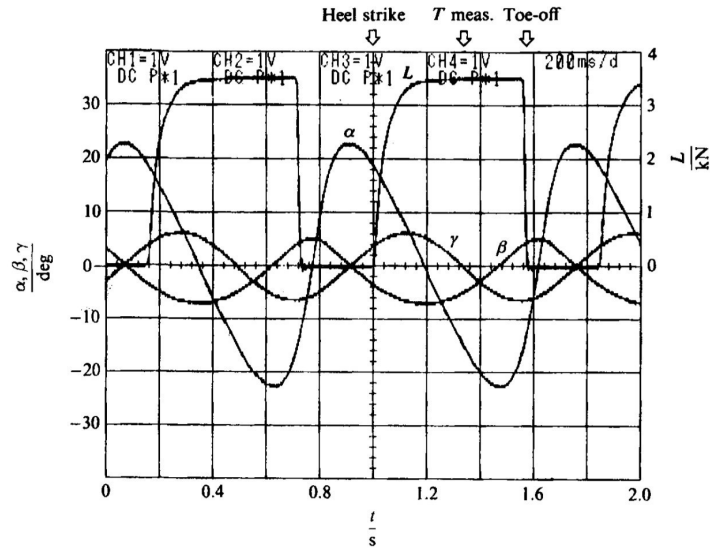


Figure 6.4: Measured variation of flexion-extension angle α , abduction-adduction angle β , internal-external rotation angle γ and load L with time t

Step 2: Digitization and Import

The “screenshot” is then digitized, or converted to a set of coordinates, using a digitizing tool. The freely available, open-source tool Engauge Digitizer was used in this work. Figure 6.5 shows the digitized data.

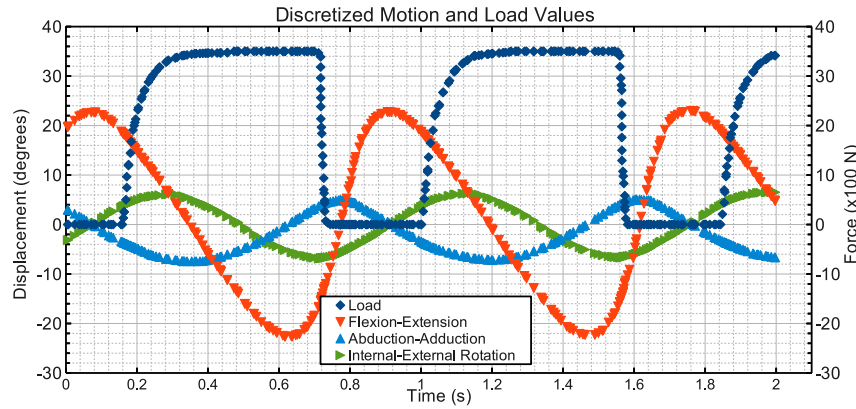


Figure 6.5: Data obtained from cite j_0 after digitization

Step 3: Curve Fitting

The digitized set of values thus generated represent “steps” in the gait cycle which would be repeated during walking. A periodic function is then fit over these discrete values to achieve repetition over different steps. This step was conducted in MATLAB. A third order Fourier series is fit to the flexion-extension motion, and a first order sinusoidal function is fit to the abduction-adduction and internal-external rotation, each. The load pulse is broken into four components: unloaded, load rise, constant load, and load drop. These four steps are repeated to represent the four phases during the load cycle, at every gait step. Smooth curves are fit independently for each of these four components, while ensuring curve continuity. Figure ?? shows the curve fitted data .

Step 4: Differentiation

The fitted curves obtained above represent the angular displacements during the three motions. These displacements are useful for the model as they represent the variation

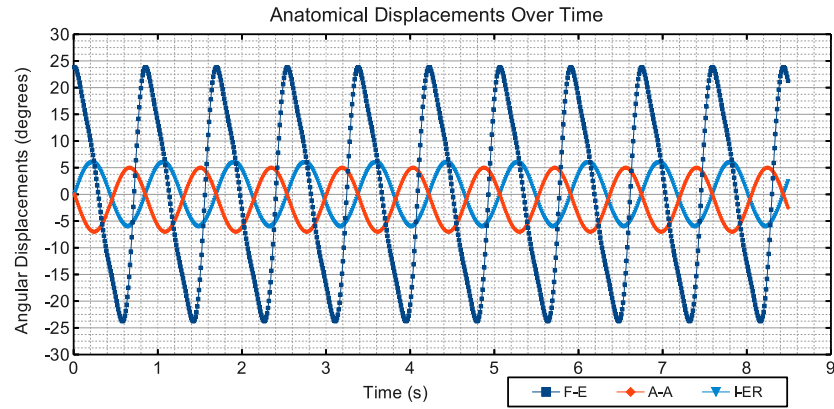


Figure 6.6: Curve-fitted, digitized data

in the contact between the femoral head and acetabular cup asperities. However, the fluid model, based on the principles of lubrication, requires entrainment velocities to calculate the load carrying capacity of the fluid. The displacement profiles are then differentiated to calculate the angular velocities during the three motions. Figure 6.7 shows the differentiated, velocity profile.

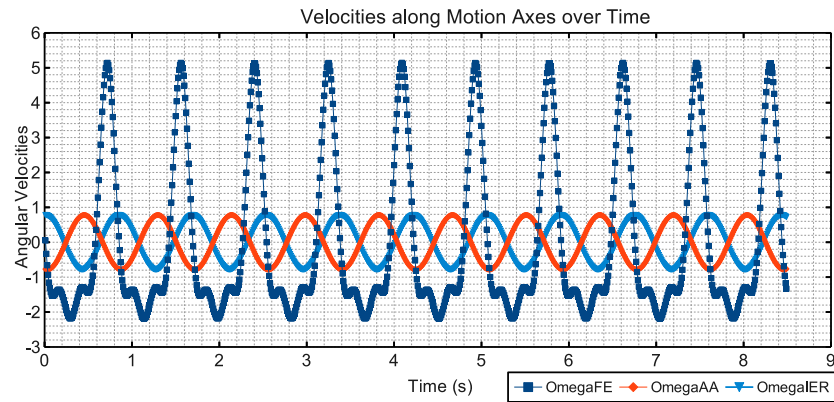


Figure 6.7: Angular velocities obtained after differentiating the displacement curves

Step 5: Coordinate Transformation A

The velocities generated in Step 4 above are along the three motion axes. However while walking, these motion axes are not aligned to coordinate axes fixed in space. Only the I-ER axis can be assumed to be fixed to the vertical axis. Both F-E and A-A axes oscillate about the I-ER axis, and their displacement is the same as the I-ER displacement (γ). Even though the A-A axis oscillates about the I-ER axis, it always remains orthogonal to the I-ER axis. The F-E axis on the other hand oscillates about the A-A axis as well, with the displacement the same as the A-A displacement. The F-E axis thus, remains orthogonal to neither I-ER axis, nor the A-A axis. Figure 6.8 shows the two sets of coordinate axes: the F-E, A-A and I-ER axes, that represent the directions of motion; and the medial-lateral, superior-inferior, and anterior-posterior axes that are associated with the human anatomy and thus assumed to be fixed in space. Figure 6.9 shows the transformed velocities along the anatomical coordinate axes.

The load, on the other hand, is applied on the acetabular cup, which can be assumed to remain stationary with respect to the anatomical coordinate axes. Thus the direction of the applied load remains constant over space, and is assumed to be at an angle of 45° medial to the I-ER, or superior-inferior axis. Figure 6.10 shows the forces along the anatomical coordinate axes.

Step 6: Coordinate Transformation B

After Step 5 above, we get velocities aligned through a stationary set of coordinate axes. However, since the acetabular cup is inclined to the vertical at a angle of about 45° , the axes of the tribological interface are not aligned with the anatomical axes.

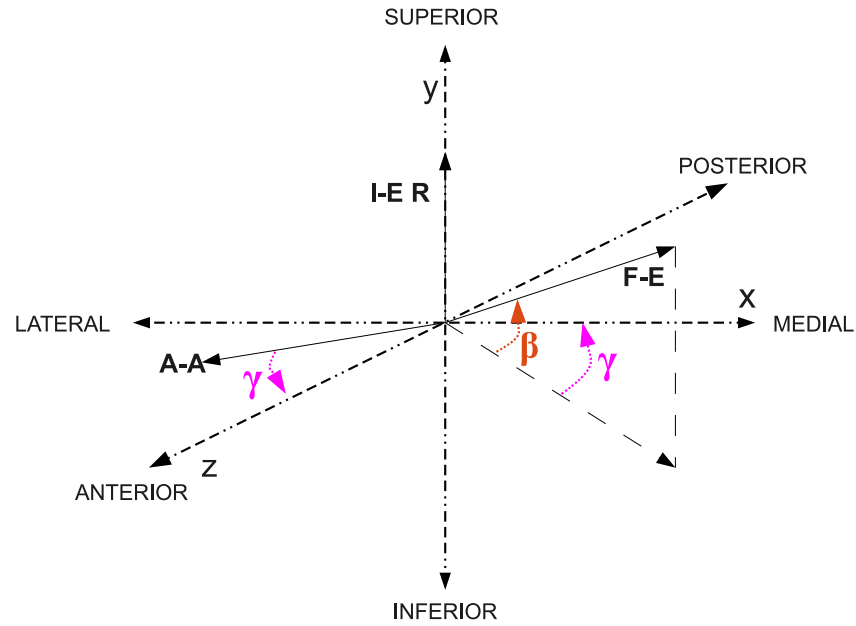


Figure 6.8: The two sets of coordinate axes: motion, and anatomical

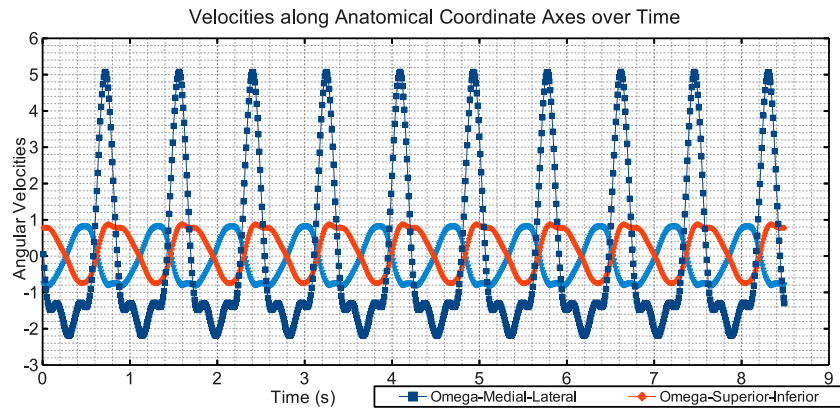


Figure 6.9: Velocities along the anatomical coordinate axes, obtained after transforming the velocities along the motion axes

Another coordinate transformation is conducted to obtain the angular velocities and forces along the tribological axes. Figure 6.11 shows the velocities, and fig. 6.12

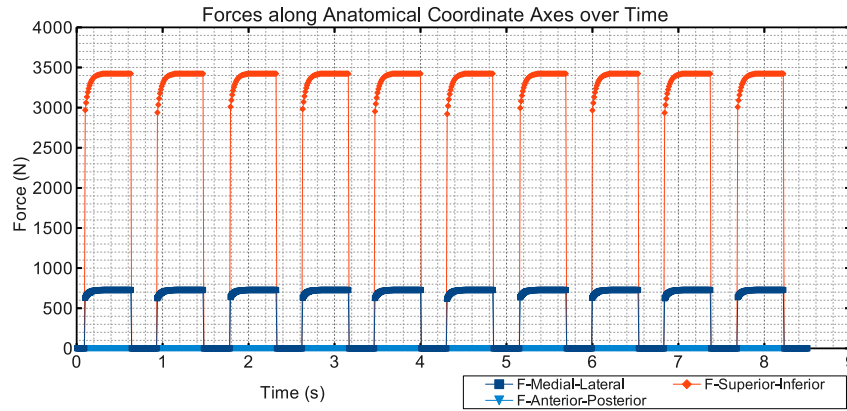


Figure 6.10: Forces along the anatomical coordinate axes, obtained after taking the components of the applied transient load along the anatomical axes

shows the forces, along the tribological coordinate axes. These transformed values of angular velocities and forces, are then ready to be used in the model discussed in the previous sections (6.2)

Figure 6.11 summarizes the three angular motions, the load, and three sets of coordinate axes.

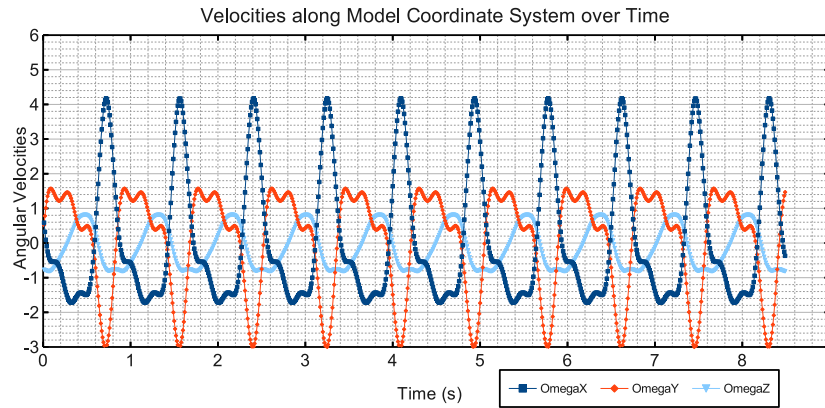


Figure 6.11: Velocities along the tribological coordinate axes, obtained after transforming the velocities along the tribological axes

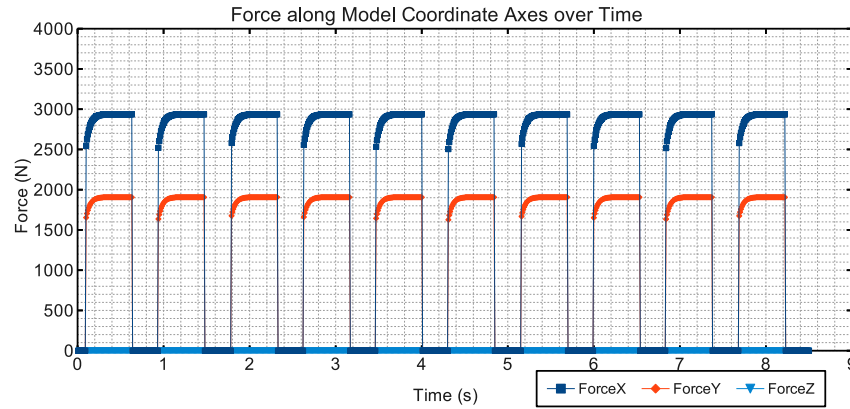


Figure 6.12: Forces along the tribological coordinate axes, obtained after transforming the anatomical forces along the tribological axes

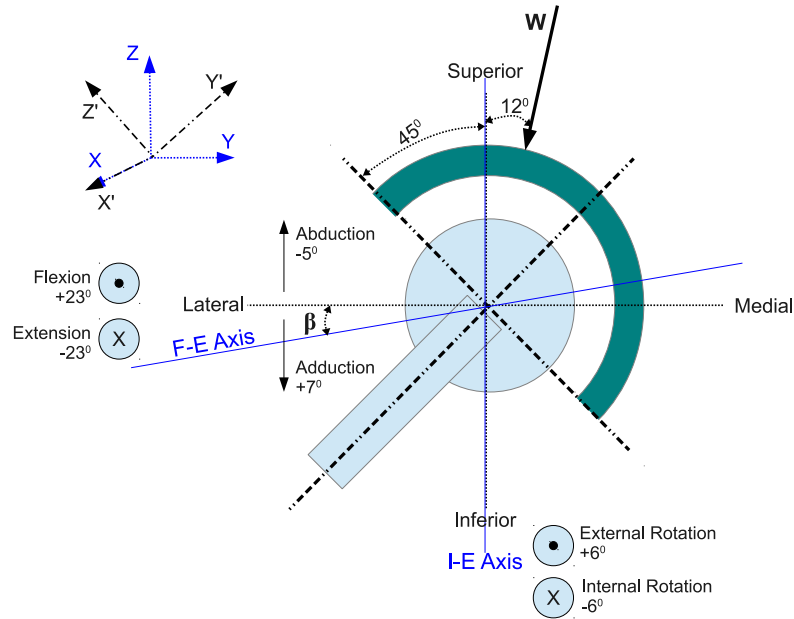


Figure 6.13: Summary of the motion and loading of the hip joint. Notice the three sets of coordinate axes: along the motion (flexion-extension, abduction-adduction, internal-external rotation), along the human anatomical axes (medial-lateral, superior-inferior, anterior-posterior), and along the tribological axes (X' , Y' , Z')

6.3.2 Lubrication fundamentals

In tribology, an interface can operate in three different lubrication "regimes", that differ in their mechanism of supporting the load. The regime of operation of a typical system can be identified by its operating conditions, namely the load, relative velocity between the surfaces and viscosity of the fluid. The three regimes are known as boundary or dry lubrication, the hydrodynamic or full-film lubrication and mixed lubrication. Dry lubrication regime has almost no role of the fluid lubricant and the entire load is supported by the two solid bodies in contact. In full-film lubrication, there is virtually no contact between the two solids and the entire load is supported by the fluid film. The mixed lubrication falls between these two extremes and here the load is being shared by the solid-solid contact and the fluid lubricant.

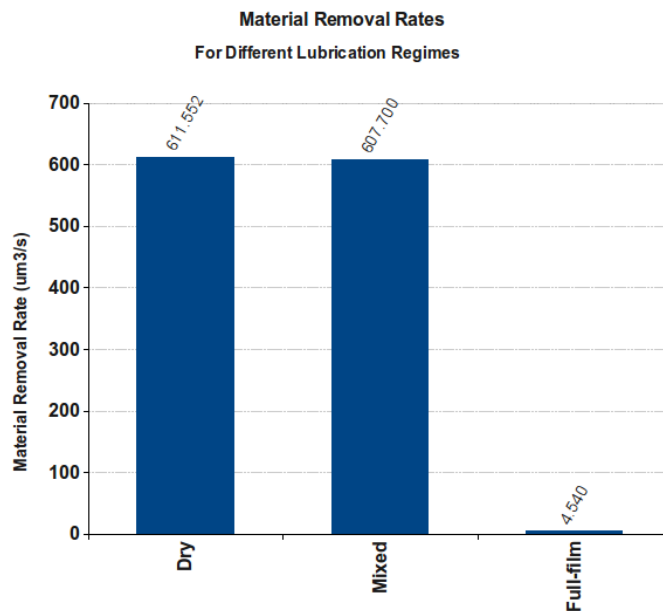


Figure 6.14: Material removal rate with different lubrication regimes

It is intuitive that dry lubrication would lead to much higher wear and friction resistance. On the other hand, in extreme cases, even full-film lubrication would cause higher friction because of high viscous resistance from the fluid lubricant. However, there would be virtually no wear, as the primary cause of wear is abrasion or adhesion between the solids. Thus operation in mixed lubrication seems to be a promising situation where one can expect lesser friction and slightly lesser wear than dry lubrication. This phenomenon is easily illustrated in figure 6.14 which compares wear rates in the three regimes for a hypothetical hip-joints that can operate in all three regimes. In reality, the conditions during the operation of the hip joint cause it to operate in the boundary lubrication regime (the velocity is low, the load is high and lubricant has low viscosity). As fig. 6.14 suggests, it would be ideal to have a hip-joint that operates in the full-film lubrication regime, however obtaining such conditions in a typical joint is virtually impossible. However, it is possible to push the operation to mixed lubrication and achieve lesser wear. Texturing the surface is one of the effective alternatives that reduce the wear by pushing the system from boundary to mixed lubrication, as will be shown here.

6.3.3 Equilibrium orientation

As mentioned earlier, the quasi-equilibrium orientation provides us the three eccentricity values: e_x , e_y , e_z in the x , y and z directions respectively. These orientation parameters can then be used to observe the temporal evolution of fluid pressure in the cup-head interface. This can help us understand the tribological regime the hip joint operates under, in a typical gait cycle. Similarly, in a simulated gait cycle, a time evolving cup-wear map can be constructed to determine the sections of the acetabular cup that undergo the highest amount of wear, to optimize the topography

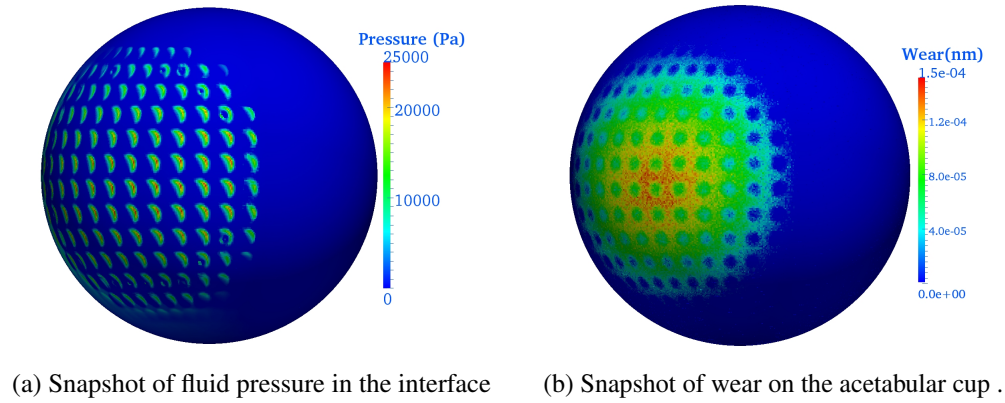


Figure 6.15: Sample output profiles from the model

of the cup for minimal wear. Figures 6.15a and 6.15b show such sample fluid pressure field and wear map over the acetabular cup.

6.3.4 Wear

The model can be used to study the variation in material loss as a function of a variety of parameters, that act as an input to the model. One such popular parameter is the size of the femoral head. There has been significant debate around the ideal size for the replacement femoral head. It has been argued that larger heads result in “shallower” wear scars, thus retain their tribological performance for longer periods. However, together with shallower wear scars, larger heads also result in higher wear volumes, thus generating a larger quantity of wear debris. As has been mentioned previously, higher concentration of wear debris would result in faster onset of osteolysis, thus reducing the life of the joint. Because of this conflict in performance of femoral heads of different sizes, several authors have studied the wear performance of femoral heads as a function of the head size.

The wear predictions of the current model have been compared against experimental

results published by Livermore et al. [117] where they conducted radiological measurements of acetabular cup wear, and other numerical analyses by Maxian et al. [118, 119] and Wu et al [120].

Figure 6.16 compares the volumetric wear of the present model with the experimental measurements conducted by Livermore et al. and the predictions of Wu et al.'s FEA model. It can be seen that the current model matches well with the experimental measurements, and excellently with Wu's model. This shows that even though the present framework utilizes lower order models for its contact mechanics and hydrodynamic effects, the coupled effect of these mechanisms is accurately captured.

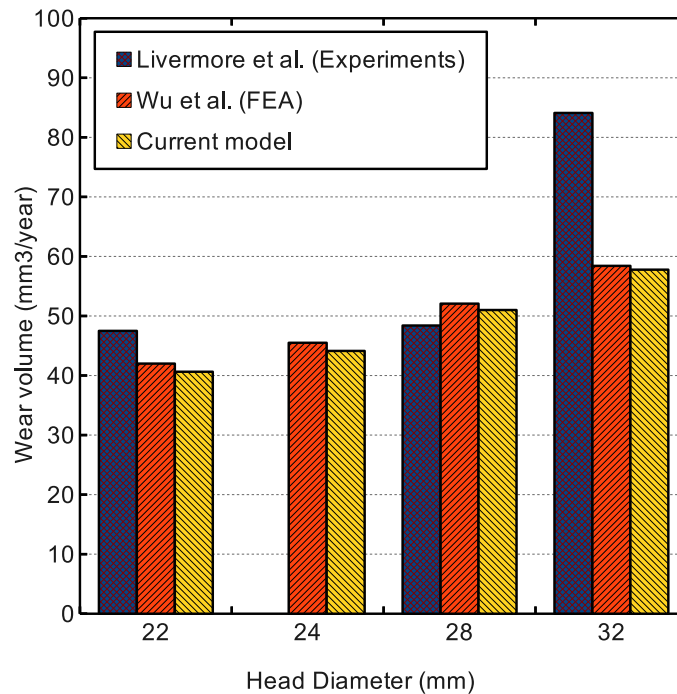


Figure 6.16: Variation of volumetric wear with the size of the femoral head

Figure 6.17 compares the radial wear rate among the same models and experiments as in the previous case of wear volume. The predictions of Maxian et al.'s model have been added to this study, as they presented one of the earliest, widely accepted models for prediction of acetabular cup wear. Even though the match between the present model's predictions and the experimental measurements is not as good as the wear volume, differences are small. While trend-wise similarity can be clearly observed, quantitatively the model under-predicts the wear rate. However, it is important to point out the difference that the experimental measurements refer to the maximum wear-rate over the entire cup, whereas the model plots the "average" wear rate across the entire cup. In the near future, the comparison of maximum wear rates between the model and experiments would prove to be more accurate.

6.3.5 Parametric studies

Since the accuracy of the model predictions was tested by comparison against experiments, the model was then used to conduct parametric studies to investigate problems that are difficult, or almost impossible to solve experimentally. One of the primary problems that has been left unsolved is to study the effect of different surface texture patterns on the tribological performance of the artificial joint.

The surface texture is defined through several parameters: shape of the texture, depth of the texture, radius of the texture, separation of the texture to name a few. Figure 6.18 shows a textured surface with different parameters marked. Parametric studies were conducted to study the effect of certain surface texture parameters on final concentration of the debris in the synovial fluid. The shape of the textures was kept spherical for all studies.

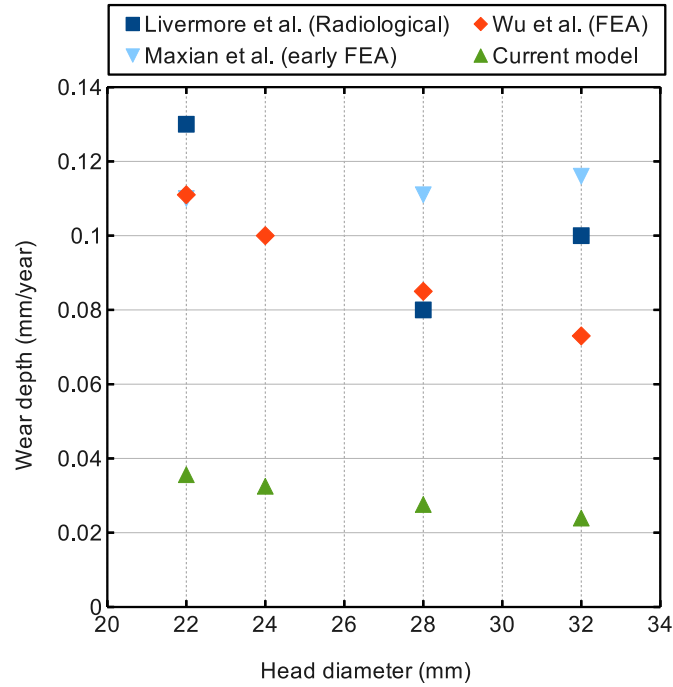


Figure 6.17: Variation of wear rate with the size of the femoral head

Texture Depth

The effect of varying texture depths for a constant texture width was studied. This was achieved by changing radii of the spherical textures, as shown in fig. 6.19a. Figure 6.20 shows the variation of the instantaneous material removal and material deposition over time for a single gait cycle, for different texture depths.

It has been hypothesized earlier that the hip-joint is operating in the boundary or mixed lubrication regime. In those regimes, as majority of the load is being carried by the solid-solid contact pressure, there is almost no variation in the average contact stress over time. Following Archard's wear law (eq. (6.6)), if everything else is held constant, the wear volume should follow the same trend in relative velocity. The

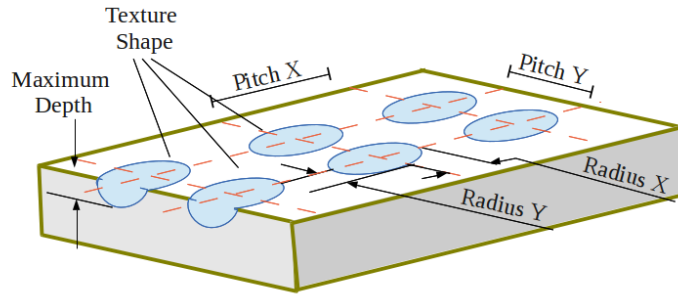


Figure 6.18: Parameters required to define the surface texture

same effect can be noticed that for all textures where the instantaneous material removal follows the variation in the velocity.

On the other hand, the deposition follows somewhat of an inverse relationship with relative velocity, as shown in fig. 6.20b. At higher relative velocities, the fluid in the interface has a higher average velocity. Under such conditions, the particles have a higher tendency to be transported by advection as compared to diffusion. Following Yew et al.'s [116] algorithm, lower diffusion leads to lower material deposition. On the other hand, at the extremes of the swing phase in the gait cycle, the rotational velocity of the head goes to zero. In absence of an entraining velocity of the solid, the fluid would nearly come to rest, leading to a much higher diffusion, and as a result, a much higher deposition of the material.

Figure 6.21 plots the aggregate quantities at the end of the gait cycle. For a constant surface radius, increase in the texture depth leads to more material being removed. This would mean that increasing the depth causes increase in the contact stress,

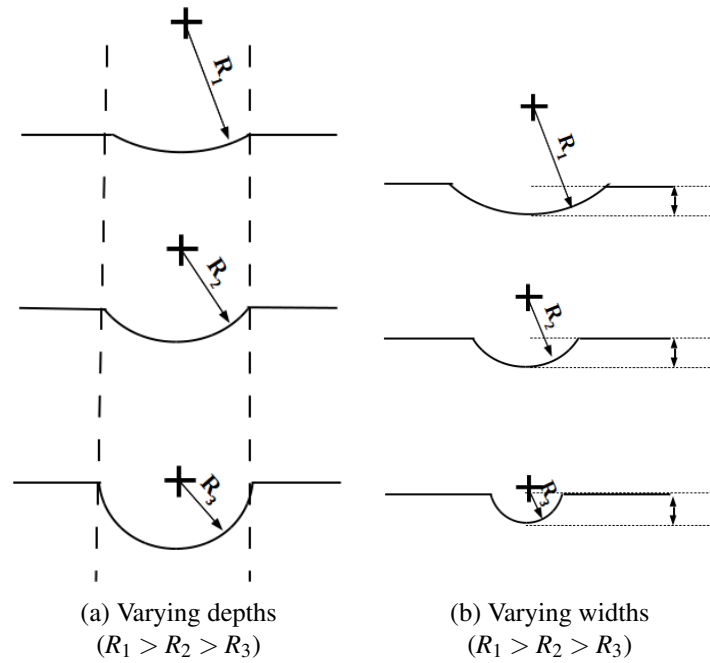
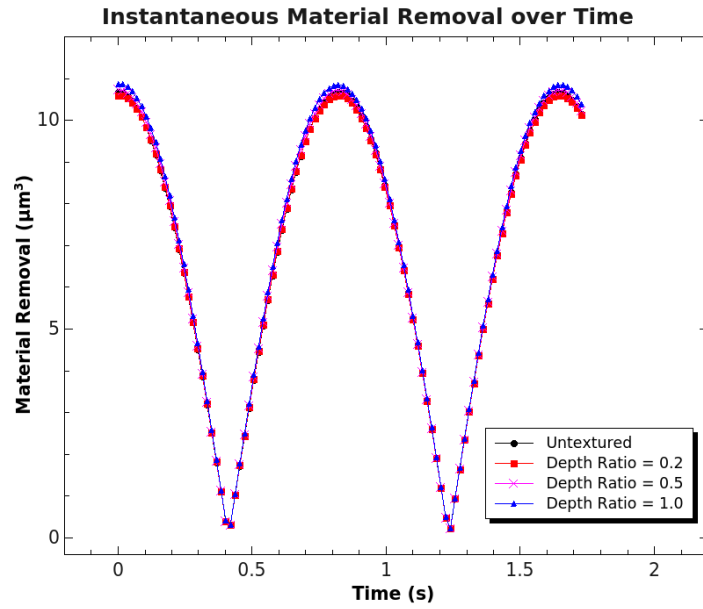


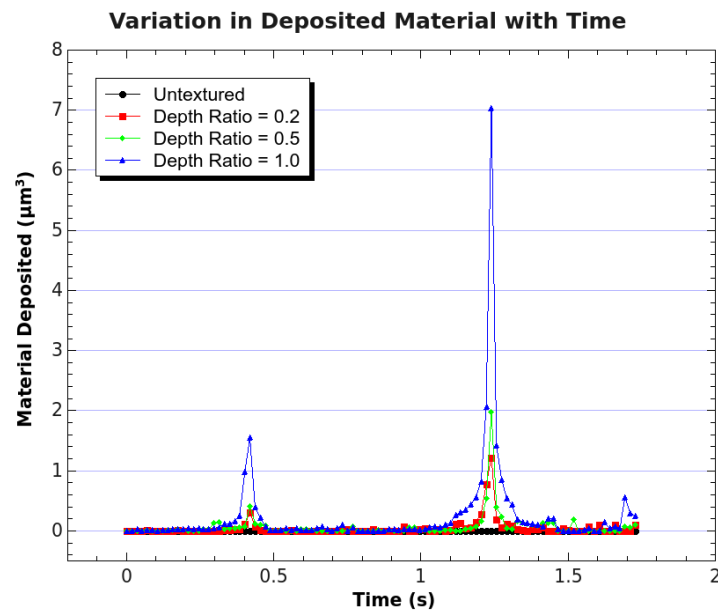
Figure 6.19: Variation in texture parameters

fig. 6.21a. This is reasonable, as upon increasing its depth, the fluid film thickness near the texture increases and lesser hydrodynamic pressure is generated within the texture. (following Reynold's equation (6.1), $p \sim 1/h^2$). Thus, lesser overall load carrying capacity is provided by the fluid, resulting in higher contact stresses and hence, more wear. Interestingly, the lowest depth textures perform better than the untextured sample showing that the for lower depths, fluid film lubrication is enhanced. Whereas for very deep textures, the lubrication film is broken at the textures resulting in loss of lubrication and more material removal.

However, as shown in fig. 6.21b, the deeper textures also lead to more mate-



(a) Instantaneous material material removal



(b) Instantaneous material deposition in the dimples

Figure 6.20: Instantaneous material removal, deposition over time

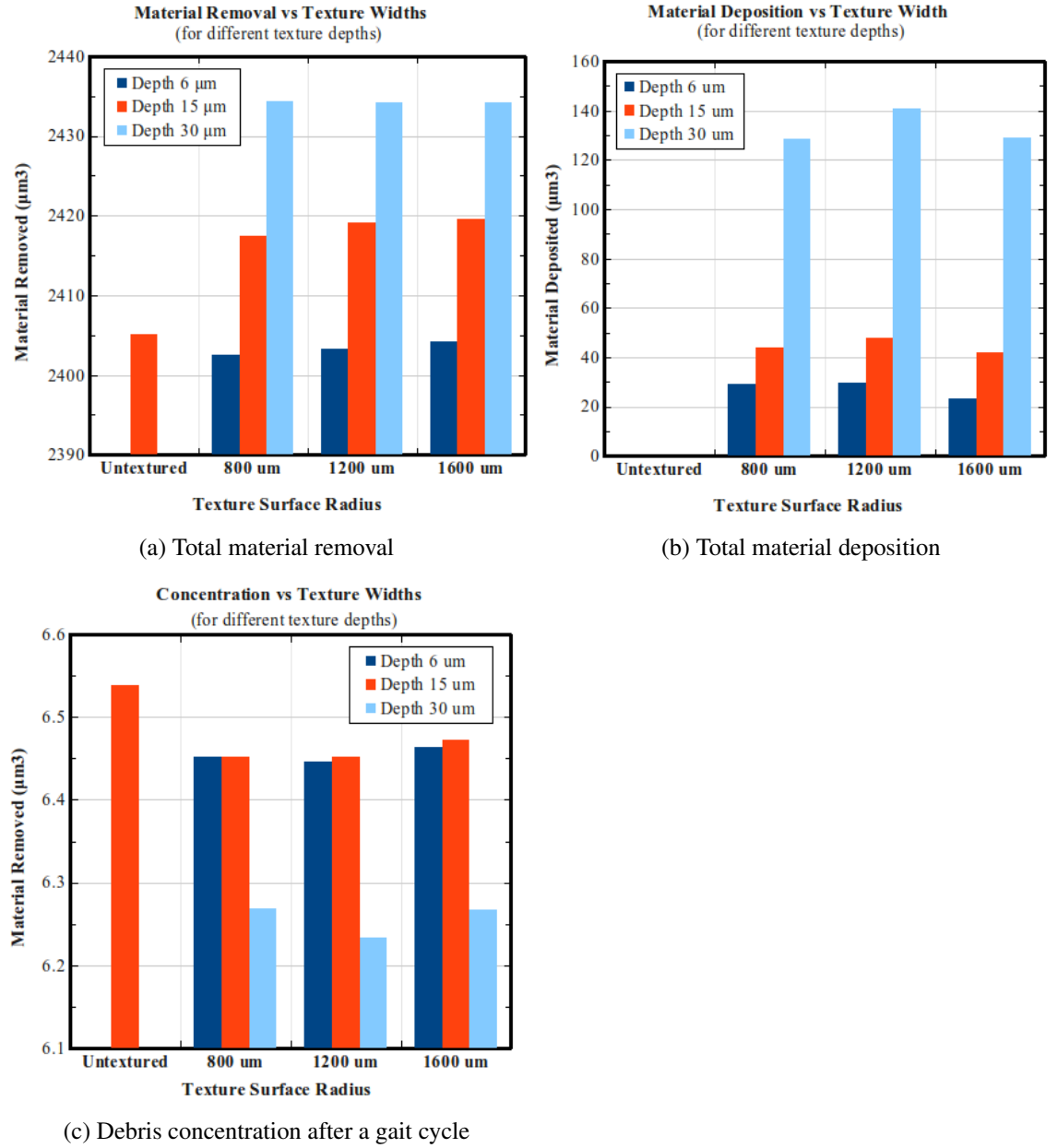


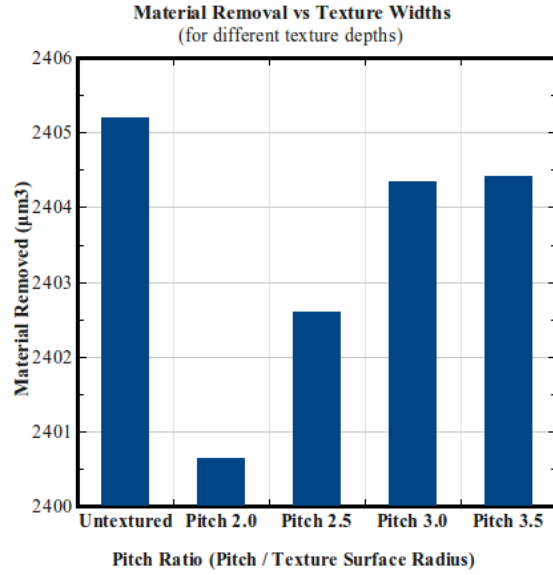
Figure 6.21: Effect of surface texture radius and maximum texture depth

rial deposition. This is also understandable, as deeper textures hold a larger volume of the lubricant, leading to a larger fraction of the fluid having Peclet numbers below the threshold limit. Thus, a larger volume of particles diffuses towards the bottom of the textures.

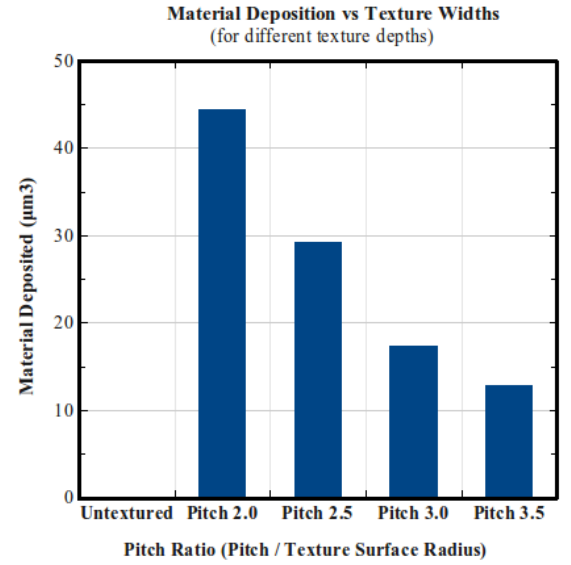
By combining the evaluations of total material removal and total material deposition, a final concentration can be calculate for different texture depths (fig 6.21c). It can be observed that the deepest textures result in the lowest concentration. This means that among the different texture depths, the difference in the material deposition is much more severe than the difference in material removal. Or, alternatively, the additional lubricating effect of the textures does not change as much with varying the texture depths, as the diffusive transport within the textures. Although the deepest textures have much larger material removal when compared with the untextured sample, they also have a significant amount of material being deposited, the resulting concentration being lesser than the untextured sample.

Texture Surface Radius

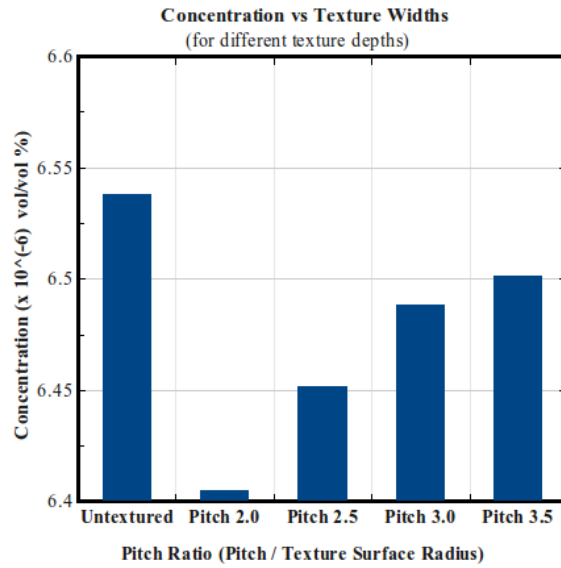
For this study, the texture depth was held constant, and by changing the radii of the textures (fig. 6.19b), the surface radius or the width of the texture was varied. The pitch ratio (texture pitch / texture radius) has also been kept constant at 2.5 to keep the influence region of an individual texture proportionate. Again, fig 6.21a shows the variation in the material removal for different texture widths. It can be seen that the material removal does show much difference by changing the texture width. The slight increase in the material removed for the shallower textures ($6\mu m$ and $15\mu m$) indicates the action of a similar phenomenon as while



(a) Total material removal



(b) Total material deposition



(c) Debris concentration after a gait cycle

Figure 6.22: Effect of separation between the textures (texture pitch)

increasing the depth. That is, by increasing the texture width one is increasing the region that has a thicker fluid film, this reducing the aggregate load carrying capacity of the fluid. This again results in higher contact stresses and higher material removal.

Material deposition has an interesting trend. Maximum material deposition is observed at an intermediate value of $1200\mu m$ radius. Consider again the volume of fluid having the Peclet number value lesser than the threshold. As the pitch ratio is held constant, the area fraction of the textures on the surface remains constant. Hence, for shallower textures, there is not much difference in the fraction of the fluid in the textures that have Peclet number less than the threshold. However, for the deeper texture (depth of $30\mu m$) the model shows that the is largest volume of almost stationary fluid occurs in the case of the $1200\mu m$ texture width.

As there was not much difference in the material removal or material deposition across the texture widths for shallower textures, the final concentrations are also pretty similar (fig. 6.21c). Material removal for deepest texture was also similar across different texture widths. However, there was significant difference in the deposited material for the deepest texture, the maximum occurring at the texture width of $1200\mu m$. As a result, for the same texture design we see the minimum concentration across the entire set of textures.

Similar to the previous study, as there is no material deposition in the case of untextured sample, the resulting concentration is higher than the textured samples.

Texture Pitch

As shown in fig 6.19, pitch is defined as the distance between the centers of two neighboring textures. The pitch ratio (pitch/ texture width) has been kept constant for all the previous studies. For this study, the texture width and depth were held constant at $800\mu m$ and $6\mu m$ respectively and the effect of variation of the pitch ratio was studied. These values for the width and depth have been chosen as they showed the highest enhancement in the fluid film lubrication. Figure 6.22a shows the variation in the material removal with increasing the pitch. Increase in the pitch increases the material removal, as it reduces the lubrication enhancement due to the presence of the textures. The material removal for the largest pitch is still less than the untextured sample. Material deposition shows an expected trend. For lower pitch values, as the area fraction of the textures on the surface is higher, we have a larger volume of fluid inside the textures. As a result, a larger fraction of the suspended particles is deposited. Finally, as the smallest pitch generates the least material, and also traps the largest fraction of the generated particles, it maintains the lowest concentration of the debris in circulation.

6.3.6 Model Limitations

The biggest limitation of the model, still, is the speed of execution. The lifecycle of an artificial hip joint is several years, which translates to several million motion cycles. The current model, while being several orders of magnitude faster than previous models, is still unable to compute more than a few tens of cycles in realistic time scales. Thus, the lifetime predictions of the model are still based on the extrapolation of the values of these limited computations. Several factors, which remain

insignificant over the simulated, smaller time scales become highly significant over the larger time scales (years). Such parameters include, but are not limited to, the evolution of surface topographies, effect of solid particles on the fluid, the “filling up” of dimples with the debris particles. Simple data extrapolation, as has been done in this study, neglects the effect of these parameters which can significantly alter the lifetime prediction. However, it can be reasonably expected that the designs that wear faster, would lead to shorter lifetimes. As a result, rather than comparing lifetime predictions, the model is ideally suited to conduct comparative studies of wear-rates among different designs.

The model assumes the behavior of the synovial fluid is governed by the steady state Reynolds equation. As a result, the model is unable to capture the temporal effects generated through the squeeze film term. Although this approximation reduces the computational cost of executing the model, the model does have to make compromises with the accuracy. The squeeze film effects become increasingly important at very low speeds, when the entire load carrying capacity, if any, from the synovial fluid is generated through the normal squeezing of the fluid. Such conditions arise at either extremes of the gait cycle. The importance of the squeeze film effects is even more important while considering the textured femoral head surfaces. Without the squeeze film effects, the model assumes that the fluid becomes stationary at the ends of the gait cycle, leading to the particle motion being dominated by Brownian diffusion. As a result, a large fraction of particles in the suspension settles down in the dimples. With the squeeze film effects, the fluid would still experience some motion at either extremes, thus leading to higher particle transport by drag, and as a result, a lower fraction of particles depositing in the dimples or reservoirs.

6.4 Conclusion

A particle augmented mixed lubrication (PAML) model was presented for a metal-on-polymer hip replacement. The model takes real surface topography as an input and can track the evolution of the fluid pressure and the material removal under realistic walking conditions. The effect of texturing the metallic femoral head was studied. The following conclusions can be made:

- Surface texturing can lead to lower material removal and debris generation under certain conditions, by enhancing lubrication
- If engineered correctly, concave textures help trap the debris and prevent them from re-entering into circulation
- Textured surfaces lead to lesser final concentration of the synovial fluid, thus reducing the probability of osteolysis
- Lower separation between the textures (pitch) and larger depth lead to lower concentration. However to achieve the lowest concentration, the texture width needs to be engineered according to the process

Chapter 7

Applications: Mechanical Seals Model

Note: The model described in this chapter has been filed as an intellectual property by Carnegie Mellon University (CMU). Any for-profit use of the modeling approach described herein requires contacting the CMU Center for Technology Transfer and Enterprise Creation (CTTEC)

7.1 Introduction

A key component of the reactor coolant system found in nuclear power plants is the reactor coolant pump, which provides a forced-circulation flow through the nuclear core in order that there is adequate heat transfer to maintain a departure from nucleate boiling ratio of greater than 1.3. Within each reactor coolant pump is a shaft seal assembly containing three seals whose function is to provide essen-

tially zero leakage along the pump shaft to the containment atmosphere during normal operating conditions. The first of these seals in the reactor coolant pump is a controlled leakage, film-riding seal whose sealing surfaces do not contact each other. Figure 7.1 shows a schematic of the first seal assembly. High pressure fluid interacts with these solid seal components, which results in a low pressure fluid exiting this stage of the seal package at a user-specified flow rate. In recent years, several comprehensive thermoelastic hydrodynamic models have been developed in order to better understand the various engineering mechanisms that are present in this problem and ultimately affect seal performance [121–131]. Results from these models have shown that film thicknesses are dependent on a number of factors, including: surrounding fluid pressure, surrounding fluid temperature, shaft rotation speed, and fluid inertia. Additionally, some of these models have been able to look at the effect of the O-ring, double-delta channel seal, and material properties on seal performance.

Comprehensive thermoelastic hydrodynamic models have to be able to describe: a) changes to the seal gap geometry due to the solid components, b) fluid pressure and temperature within the gap, and c) the interaction between pressure and solid components. Fluid pressures were obtained from the solution of either the Reynolds equation, Navier-Stokes equations, again through finite difference or finite element techniques. In order to capture effects due to the solid, the most common approach is to use the finite element method [124, 131–133]. However, the high resolution finite element simulations are computationally very expensive. Due to these computational limitations, many investigators simplified the analysis of the interaction between the fluid and solid by using influence coefficients obtained

from a preliminary set of FEM computational runs, which restricted their combined frameworks to the set of boundary conditions used in the preliminary FEA runs. In light of these shortcomings related to using FEA, some other investigations have used analytical or simplified approaches [127, 128] to simulate the solid components. However their analysis made several assumptions regarding the behavior of the solids. One major assumption made in [128]’s work was that while loaded the solid rotates about its centroid instead of bending or deforming about its supports. Such drastic approximations again limited the applicability of their modeling approach to a very specific set of conditions.

The aim of this paper is to analyze the influence of thermal and mechanical deformation of the seal face plates on the leakage rate during the start up or pressurization (i.e. increasing the pressure from ambient to the operating value) process. A thermoelastic hydrodynamic lubrication (TEHL) model is introduced that is presented as a compromise between highly accurate, but very expensive FEA models, and, faster, but approximated analytical models. Instead of using comprehensive two-dimensional FEA to analyze the deformation of solid under the fluid pressure, a semi-analytical approach, based on the theory of annular plates has been introduced that allows flexibility in load and boundary conditions while still being computationally efficient.

The rest of the paper is organized as follows. The modeling scheme is presented in the next section. The details of the lubricant modeling, solid component modeling, fluid-solid coupling, and seal operation in the balanced mode are presented. Next, the results of the TEHL model, and an isothermal, elastohydrodynamic lubrication

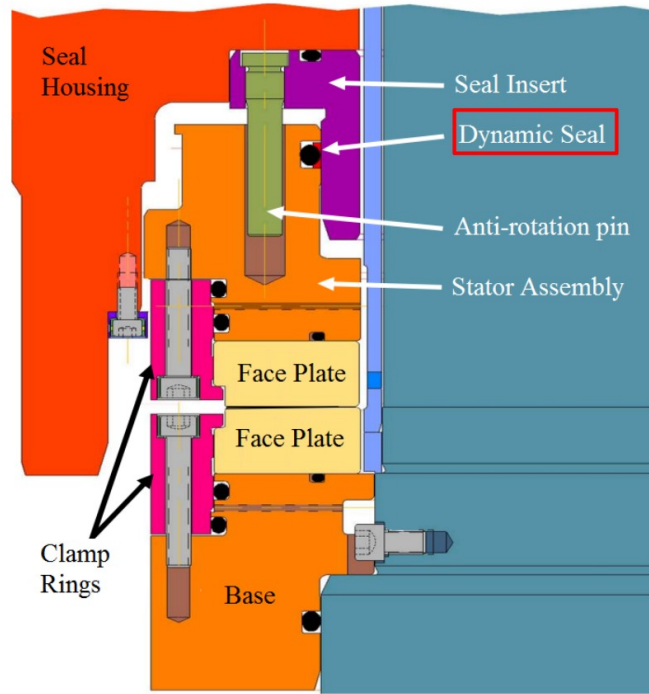


Figure 7.1: The assembly for the No.1 seal in a reactor coolant pump. The coolant flows from a high pressure region to a low pressure region, between the two face plates

(EHL) model are compared against published results. Upon experimental validation, to differentiate between the effects of thermal and mechanical deformation, the influence of several operating parameters on leak rate during pressurization is studied through both the EHL and TEHL models.

7.2 Modeling Scheme

The philosophy of the proposed modeling scheme has two parts: determining the equilibrium configuration of the flexibly mounted stator over the rotor, and

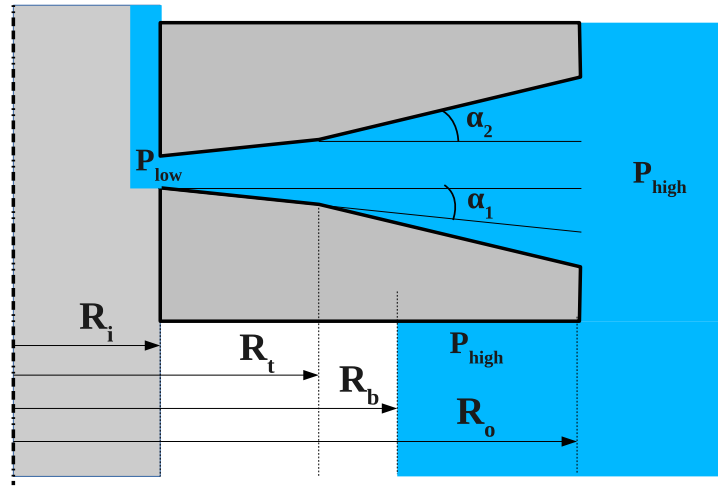


Figure 7.2: A schematic of the system being solved. The fluid flows from a high pressure region at R_o to a low pressure region at R_i through the gap between the two face plates. The fluid causes thermo-mechanical deformation in the surrounding face plates that have double- tapered geometry with minor and major taper angles as α_1 and α_2 respectively. The pressure within the seal gap is balanced by the closing load at the back of the seal assembly where the high pressure and low pressure regions are separated through the double-delta channel seal at the radial location of R_b

calculating the leak-rate in that orientation. The major forces acting on the flexibly mounted stator during operation are the hydrodynamic pressure applied by the lubricant, the weight of the stator, the friction force at the double delta channel seal, and the hydrostatic pressure of the surrounding fluid. The fluid flow is assumed to be incompressible, Newtonian and laminar, the face plate material is assumed to be linear-elastic and isotropic. Based on these assumptions, a comprehensive model is presented here that accounts for the effect of the working fluid, deformation of the face-plate, and resulting leakage through the seal. Figure 7.2 shows a schematic of the system being modeled. The following sections describe the major components of the model.

7.2.1 Fluid (hydrodynamic) modeling

The seal is assumed to operate in full film lubrication regime, i.e. the two face plates are always separated by a non-zero gap, and no solid-solid contact exists between the two surfaces. This fluid film is shown to be of the order of tens of microns, leading to lower Reynolds numbers. The surfaces of the face plates are also ground to very low roughnesses, with Ra values close to 100 nm. Although, later in the lifecycle of the seal, deposition of particulate matter can cause the roughness to increase locally, which may generate some localized turbulent flow. The fluid flow can thus be assumed to be laminar in nature, with the thin flow domain confined by the two face plates. The average flow Reynolds equation [eq. 7.1] has been used to model the flow of the fluid.

$$\frac{1}{r^2} \frac{\partial}{\partial \theta} \left(\Phi_{\theta} h^3 g \frac{\partial \phi}{\partial \theta} \right) + \frac{1}{r^2} \frac{\partial}{\partial r} \left(\Phi_r r h^3 g \frac{\partial \phi}{\partial r} \right) = \lambda \left(\frac{\partial (\phi \bar{h})}{\partial \theta} + \sigma \frac{\partial (\phi \Phi_s)}{\partial \theta} \right) \quad (7.1)$$

The equation has been solved numerically through finite differencing over a two-dimensional $r - \theta$ grid. In the radial direction, Dirichlet boundary conditions ($p = p(\theta)$) have been used for the pressure. Jacobsson-Floberg-Olsson boundaries have been used to account for possible cavitation, and ensure mass conservation through the sheared film. The reader is referred to the work of Qui and Khonsari [134] for details of numerical implementation.

The primary quantity dictating the fluid pressure (p) in the Reynolds Equation (eq. (7.1)) is the film thickness ' h '. The film thickness in this model is contributed

by three components:

$$h = h_{initial} + \delta_{mech} + \delta_{therm} \quad (7.2)$$

1. **The designed seal taper** ($h_{initial}$). The face plates have in the RCP can have up to two taper angles, on either one or both plates, creating a converging gap in the direction of the fluid flow.
2. **Mechanical deformation** (δ_{mech}). As in any typical EHL scenario, the fluid pressure can cause deformation in the surrounding solids. The face plates here deform under extreme pressures exerted by the fluid (see sec.7.2.2).
3. **Thermal deformation** (δ_{therm}). Due to extremely high shear rates, a large amount of energy is lost in the fluid in the form of viscous heat generation. This generated heat, when transferred over to the surrounding solid causes thermal expansion and resulting thermo-elastic deformation in the seal assembly sec.7.2.2).

The temperature distribution in the fluid is solved through the three dimensional energy equation, that is simplified by applying the thin fluid film assumption:

$$\rho_f C_f \left(u_r \frac{\partial T}{\partial r} + \frac{u_\theta}{r} \frac{\partial T}{\partial \theta} \right) = k_f \frac{\partial^2 T}{\partial z^2} + \mu \left[\left(\frac{\partial u_\theta}{\partial z} \right)^2 + \left(\frac{\partial u_r}{\partial z} \right)^2 \right] \quad (7.3)$$

Dirichlet boundary ($T_f = T(\theta, z)$) conditions are applied for the temperature at the radial boundaries. Axial boundary can be specified by either Dirichlet ($T_f = T(r, \theta)$) or Neumann ($q_f = q(r, \theta)$) boundaries.

7.2.2 Solid Deformation

In normal operating conditions, the seal ring assemblies will deform under the hydrodynamic pressure imposed by the fluid. These overall deformations will be dominated by the face-plate deformations if the support assembly materials are hard, and are thicker than the face-plates. It can also be assumed that under normal operation, the plates will deform axi-symmetrically.

Mechanical Deformation

Plate deformation theory is used to calculate the deformation of the annular face-plates. A brief outline of the process is given below. The reader is referred to the work of Karunasena et al. [2] for the details of implementation,

For axisymmetric bending of thin annular plates, Kirchoff (classical thin) plate theory can be used to calculate transverse deformation and slope of the plate cross section, as given by Timoshenko [135].

$$w^K = e_1 + e_2 r^2 + e_3 \log r + e_4 r^2 \log r \quad (7.4)$$

$$\frac{dw^K}{dr} = 2e_2 r + \frac{1}{r} e_3 + r(1 + 2 \log r) e_4 \quad (7.5)$$

where, e_1, e_2, e_3, e_4 are constant coefficients, and superscript K denotes quantities calculated for the Kirchoff theory.

Now, consider an annular, radial element, bound by two nodes i and j , located at $r = a_i$ and $r = a_j$. Using the above equations, the deformation and slope at nodes i and j can be written in terms of the constant e 's (following the appropriate sign

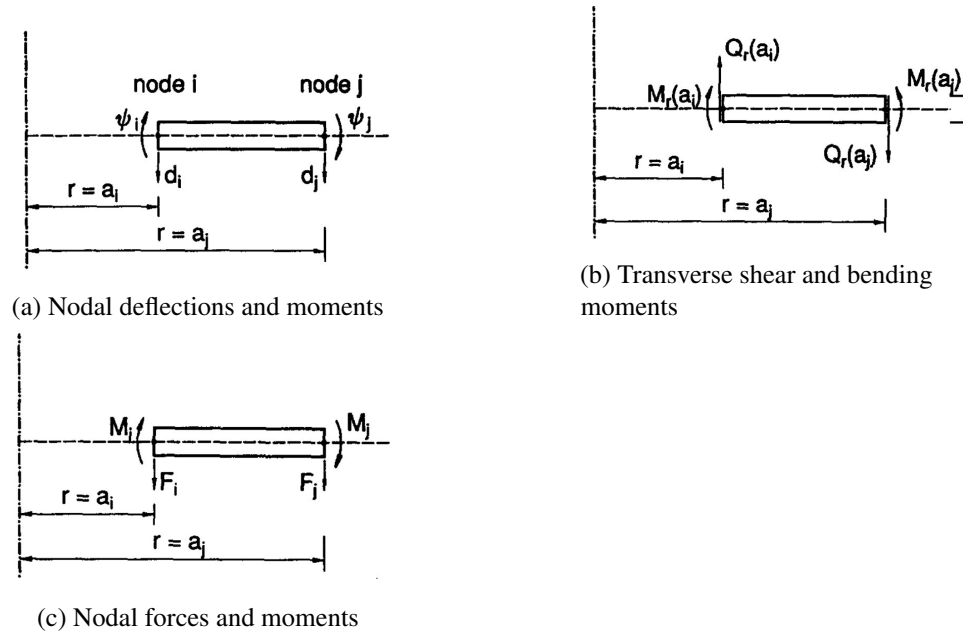


Figure 7.3: Proper sign convention for (a) Nodal displacements and slopes, (b) Transverse shear and bending moment, according to the theory of plates, and (c) Nodal forces and moments, according to finite element method; figures from [2]

convention for displacements and slopes, fig. 7.3a):

$$\mathbf{d}^K = \mathbf{A}_1 \cdot \mathbf{e} \quad (7.6)$$

$$\text{where, } \mathbf{d}^K = \begin{Bmatrix} d_i^K \\ \psi_i^K \\ d_j^K \\ \psi_j^K \end{Bmatrix}, \quad \mathbf{e} = \begin{Bmatrix} e_1 \\ e_2 \\ e_3 \\ e_4 \end{Bmatrix} \quad (7.7)$$

$$[\mathbf{A}_1] = \begin{bmatrix} 1 & a_i^2 & \log a_i & a_i^2 \log a_i \\ 0 & 2a_i & \frac{1}{a_i} & a_i(1 + 2 \log a_i) \\ 1 & a_j^2 & \log a_j & a_j^2 \log a_j \\ 0 & 2a_j & \frac{1}{a_j} & a_j(1 + 2 \log a_j) \end{bmatrix} \quad (7.8)$$

Also, given displacement w^K , transverse shear force Q_r^K and radial moment M_r^K can be given as:

$$Q_r^K = -D \frac{d}{dr} \left[\frac{1}{r} \frac{d}{dr} \left(r \frac{dw^K}{dr} \right) \right] = -4D \frac{1}{r} e_4 \quad (7.9)$$

$$M_r^K = -D \left(\frac{d^2 w^K}{dr^2} + \frac{\nu}{r} \frac{dw^K}{dr} \right) \quad (7.10)$$

$$= D \left[-2(1+\nu)e_2 + \frac{1-\nu}{r^2} e_3 - (3+\nu+2(1+\nu)\log r)e_4 \right] \quad (7.11)$$

$$\text{where, } D = \frac{Et_p^3}{12(1-\nu^2)} \quad (7.12)$$

Using the shear force Q^K and radial moment M^K , the nodal external forces F_i^K , F_i^K and moments M_i^K , M_i^K can be written as (following appropriate sign convention, fig. 7.3c):

$$\mathbf{F}^K = \begin{bmatrix} F_i^K \\ M_i^K \\ F_j^K \\ M_j^K \end{bmatrix} = 2\pi \begin{bmatrix} -a_i Q_r^K(a_i) \\ a_i M_r^K(a_i) \\ a_j Q_r^K(a_j) \\ -a_j Q_r^K(a_j) \end{bmatrix} = \mathbf{A}_2 \cdot \mathbf{e} \quad (7.13)$$

$$\text{where, } [\mathbf{A}_2] = 2\pi D \begin{bmatrix} 0 & 0 & 0 & 4 \\ 0 & -2(1+\nu)a_i & \frac{1-\nu}{a_i} & -a_i(3+\nu+2(1+\nu)\log a_i) \\ 0 & 0 & 0 & -4 \\ 0 & 2(1+\nu)a_j & -\frac{1-\nu}{a_j} & a_j(3+\nu+2(1+\nu)\log a_j) \end{bmatrix} \quad (7.14)$$

Combining equations (7.14) and (7.15) above, one can obtain:

$$\mathbf{F}^K = [S^K] \mathbf{d}^K \quad (7.15)$$

where, S^K is the Kirchoff stiffness matrix given by:

$$[S^K] = [\mathbf{A}_2][\mathbf{A}_1]^{-1} \quad (7.16)$$

F^K is the total load acting on the nodes, which is a sum of actual external nodal force, and nodal equivalent force of a distributed load over the element. For a uniformly distributed load 'q' F^K can be written as:

$$\mathbf{F}^K = \mathbf{f}^K + \mathbf{f}_0^K \quad (7.17)$$

$$\mathbf{f}_0^K = [S^K] \mathbf{d}_p^K - \mathbf{f}_p^K \quad (7.18)$$

$$\text{where, } \mathbf{d}_p^K = \frac{q}{64D} \begin{pmatrix} a_i^4 \\ 4a_i^3 \\ a_j^4 \\ 4a_j^3 \end{pmatrix} \quad \text{and, } \mathbf{f}_p^K = \frac{\pi q}{8} \begin{pmatrix} 8a_i^2 \\ -a_i^3(3+\nu) \\ -8a_j^2 \\ a_j^3(3+\nu) \end{pmatrix} \quad (7.19)$$

where, $\mathbf{f}^K$ are forces acting directly on the nodes. $\mathbf{f}_0^K$, are equivalent nodal forces of distributed loads, and can be calculated using the reaction forces for an annular Kirchoff plate with no internal support and clamped at both ends.

Similar analysis can be conducted for thick-plate, or Mindlin plate theory. The reader is referred to the work of Karunasena et al. [2] for the details of implementation.

Solid Temperatures and Thermal Deformations

With the high pressure gradients across, and consequent Couette-Poiseuille flow, the fluid undergoes very high levels of shearing within the small seal gap. This high shearing causes large viscous heat generation. As a result, the face-plates and the entire support assembly deform due to the heat transferred from the fluid to the solid.

At steady-state, the temperature distribution within the face-plates can be calculated using the two dimensional energy equation:

$$\nabla \cdot (k_s \nabla T) = 0 \quad (7.20)$$

$$\frac{\partial}{\partial r} \left(k_s \frac{\partial T}{\partial r} \right) + \frac{\partial}{\partial z} \left(k_s \frac{\partial T}{\partial z} \right) = 0 \quad (7.21)$$

The temperature distribution is calculated by using the boundary conditions as shown in fig. 7.4. At steady state, as the temperature rise across the seal is small, it can also be assumed that the material properties remain constant. Since the equation of thermo-elasticity would remain linear, one can use the influence coefficients method to calculate the temperatures and thermo-elastic deformations on the surface of the face-plates. The influence coefficient matrices are calculated by applying small perturbations to each node around an approximate equilibrium position. For a given surface flux vector q'' , surface temperature T_s and deformation u_T at node i

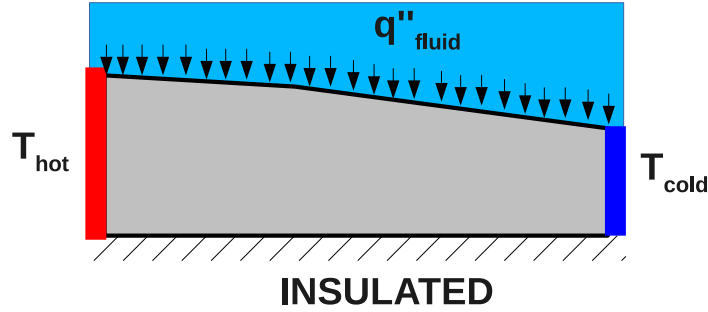


Figure 7.4: Thermal boundary conditions for the face plates. The right edge is at equilibrium with the high pressure fluid at low temperature. The fluid goes through the seal gap, experiences high shear in the gap and with high viscous heat generation, comes out at higher temperature. The left edge of the plate is at equilibrium with this heated fluid. The top edge interacts with the fluid being heated and experiences a heat exchange with the fluid in the form of distributed flux. The bottom edge is assumed to be insulated

can be given as:

$$T_s(i) = T_{app}(i) + C_{Tij} * \frac{q''(j) - q''_{app}(j)}{\delta q''} \quad (7.22a)$$

$$u_T(i) = u_{app}(i) + C_{Dij} * \frac{q''(j) - q''_{app}(j)}{\delta q''} \quad (7.22b)$$

where, T_{app} and u_{app} are the approximated temperature and deformation equilibrium positions, and are related to equilibrium thermal loads q''_{app} .

7.2.3 Coupling

Mechanical Coupling

The fluid pressure is applied directly on to the solid as a distributed, surface load. In return, the solid deformation alters the domain of the fluid flow (film thickness, in

this case).

Thermal Coupling

The thermal coupling between the solid and the fluid is more complex. A thermal equilibrium has to be maintained at the fluid-solid interface. Figure 7.5 represents this balance graphically. The fluid temperature at the interface has to be equal to the solid temperature. Moreover, in the absence of heat generation at the interface, the heat flux leaving the fluid, has to be equal to the flux entering the solid. In the present model, the solid surface temperatures are used as the axial boundary conditions for the fluid. The temperature distribution thus obtained by solving the fluid energy equation within the fluid is then used to calculate the flux leaving the fluid. This flux is used as the boundary condition for the solid heat equation, to solve for a new temperature distribution within the solid, as discussed in section 7.2.2, generating a new solid surface temperature distribution. This iterative process is repeated until convergence is achieved in the boundary temperature and flux values. Together with this thermal equilibrium, the fluid and solid are also in thermo-mechanical equilibrium. The heated fluid causes heating in the solid resulting in thermal expansion of the solid, and eventual thermo-elastic deformations at the surface of the face-plates. These thermo-elastic deformations, together with the mechanical deformations, in return, modify the domain of the fluid flow (film thickness, in this case).

7.2.4 Dynamic Balancing

Traditionally, the stator is flexibly mounted on the housing with three degrees of freedom to allow stability during operation. These are one degree of axial translation,

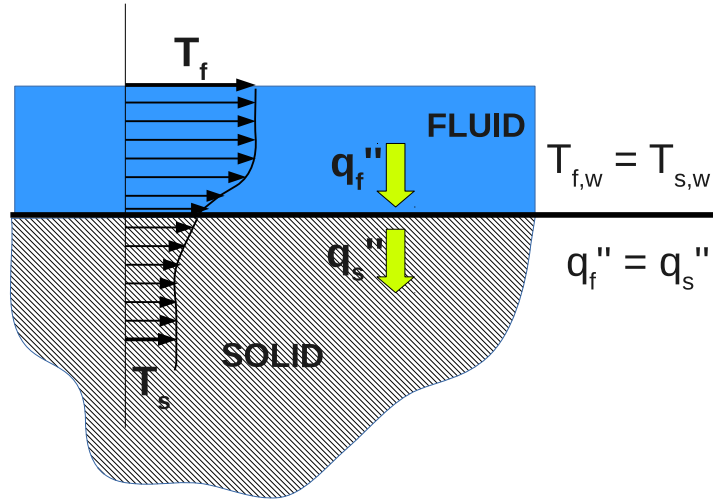


Figure 7.5: The fluid and the solid exist in a thermal equilibrium at the interface. The fluid and solid temperatures are equal at the boundary. Since there is no heat source or sink at the boundary, energy leaving the fluid should also be equal to the energy entering the solid

and two degrees of rotational misalignments along radial directions. However, for the case of perfectly aligned faces, and assuming stable operation, the three degrees of freedom have been limited to just one, in the form of axial translation. That equilibrium axial translation (h_0) is calculated by ensuring the loads on the face plates are balanced:

$$F_{opening}(h_0) + F_{closing} = 0 \quad (7.23a)$$

$$\text{where, } F_{opening}(h_0) = \int_{R_i}^{R_o} 2\pi r P(r) dr \quad (7.23b)$$

$$F_{closing} = - [\pi P_{high} (R_o^2 - R_b^2) + \pi P_{low} (R_b^2 - R_i^2)] \quad (7.23c)$$

where, $F_{opening}$ is the hydrodynamic lift force generated in the seal gap, and depends on the equilibrium axial translation, geometry of the face-plates, and their net

Table 7.1: Model Parameters

Face plate Properties	
Material	Si ₃ N ₄
Density	3.29 kg/m ³
Elastic Modulus	310 GPa
Poisson's Ratio	0.27
Thermal Conductivity	30 W/m-K
Specific Heat Capacity	711 J/kg-K
Coefficient of Thermal Expansion	3.3x10 ⁻⁶ /°C
Roughness	50 nm
Lubricant Properties	
Fluid	Water
Density	990 kg/m ³ @40°C
Viscosity	7.054x10 ⁻⁴ Pa-s @40°C
Specific Heat Capacity	4180 J/kg-K
Thermal Conductivity	0.61 W/m-K
Operating Parameters	
Inlet Pressure (OD)	15.6 MPa
Outlet Pressure (ID)	0.34 MPa
Temperature Range (OD/ID)	40/45°C
Shaft Speed	100 rad/s

deformation. $F_{closing}$ is the force of the surrounding fluid and depends only on the geometrical parameters, and operating pressures.

7.3 Results

7.3.1 Solution Procedure

Figure 7.6 shows the overall algorithm followed in the EHL model. An equilibrium axial translation (δ_0) is guessed. The film thickness is calculated using the cross-sectional geometry of the face plates. The fluid pressure p is calculated for this film thickness. The calculated fluid pressure causes some mechanical deformation

in the face plates. The mechanical deformation, in turn, modifies the gap for the fluid. The change in the gap geometry is then used to update the film thickness. The steps are repeated until consistency is obtained in the fluid pressure and mechanical deformation. This iterative process is termed as the “EHL Loop” in the flowchart. Once convergence of the EHL loop is obtained, the converged fluid pressure is used to check if the seal assembly is dynamically balanced, i.e. if eq. (7.23) is satisfied. If not, a root-finding algorithm is used to modify the axial translation (δ_0). Once the load balancing is satisfied, the steady state film thickness and leak rate are calculated.

Figure 7.7 shows the algorithm for the TEHL model. The only difference between the TEHL and EHL algorithms are in inner loops. The inner TEHL loop is a complex, coupled process instead of the sequential three step process followed in the EHL loop. Figure 7.8 shows steps involved in the inner TEHL loop. The following steps are followed to ensure convergence in the TEHL loop:

- Step 1 For a given (δ_0), the film thickness is calculated from the cross-sectional geometry of the face plates.
- Step 2 This film thickness is then used to calculate the initial fluid pressure through the Reynolds equation, eq. (7.1).
- Step 3 The fluid pressure is used to calculate the mechanical deformations and flow velocity profiles.
- Step 4 The velocity profiles, are used to calculate the fluid temperature distribution (T_f) using the energy equation (7.3). The solid temperatures are used as the axial boundary conditions.

- Step 5 The fluid temperature field (T_f) is used to calculate the flux leaving the fluid (q''_f), which is equal to the flux entering the solid. The fluid temperature distribution is also used to update the material properties (viscosity, density) of the fluid.
- Step 6 The flux field is used to calculate the solid temperature distribution (T_s), and the thermal deformation (u_T) at the solid surface.
- Step 7 The calculated solid surface temperature is then fed back to the fluid energy equation solution as a boundary condition, and Step 4 is repeated, until convergence.
- Step 8 The solid surface deformation u_T , calculated in Step 6 is combined with the mechanical deformation calculated in Step 3 to update the film thickness calculated in Step 1. The updated film thickness and the updated material properties (calculated in Step 5), are used to repeat Step 2.
- Step 9 The iterative process above is repeated until the net face plate deformation calculated using Step 3 and Step 6 remains unchanged between two iterations.

7.3.2 Numerical Accuracy

The numerical accuracy of the multi-physics, multi-platform model was assessed through grid independence studies conducted on the leak rate and equilibrium minimum film thickness. TEHL simulations were conducted for grids with number of radial elements as 34, 85, 170, 200, 250 and 340, with the axial elements appropriately scaled. Since both in house and thermo-mechanical FEA models for

deformation assume axi-symmetry, number of tangential elements is kept constant.

At low pressures, while increasing the number of elements, leak rate drops slightly from the value at the coarsest grid (34 elements), but stays virtually constant for all grids with elements higher than 85. At higher pressure gradient, there is minor change in the magnitude of the leak rate, as seen in fig. 7.9b (inset), but the percent change over varying the grid size is extremely small.

Similarly, at low pressures the minimum film thickness varies slightly while increasing the grid resolution, but becomes virtually constant above 170 elements as shown in fig. 7.10a (inset). At higher pressures, the film thickness keeps varying until 200 elements, and observes small change beyond that (fig. 7.10b, inset). The percent change in the minimum film thickness for both low and high pressures is very small, when the grid resolution is increased.

Since the simulation achieves high numerical accuracy for all grid sizes with more than 34 elements, a grid resolution of 170 radial elements was used to minimize errors.

7.3.3 Experimental Validation

The predictions of the model were compared against previously published numerical and experimental data. The comparisons are discussed in the sections below.

Pressure and Temperature

The pressure and temperature distribution in the fluid, predicted by the model was compared with the predictions of Galenne and Pierre-Danos' μ model. The pressure distribution, the drop from about 16 Mpa at the outer diameter to about 0.5 Mpa

at the inner diameter, is well matched between both models. The temperature distribution, differs slightly at the extremes, but still matches well qualitatively.

Film Thickness and Temperature Distribution

The equilibrium film thickness and temperature distribution predicted by the model were compared against Brunetiere et al.'s $\bar{\mu}$ model meant for high leakage seals. Although Brunetiere et al.'s simulated double tapered seals (i.e. both the face plates were tapered), as opposed to the present model which simulates single taper seals, the film thicknesses should remain similar. As seen in fig. 7.12, the film thicknesses for both models vary linearly from about $10\mu m$ at inner diameter to about $35\mu m$ at the outer diameter. The temperature distribution is also similar, as both models predict a temperature rise of about $7 - 8^{\circ}C$ while the fluid moves from the outer diameter to the inner diameter.

Leak rate

Galenne and Pierre-Danos reported field data from the St. Alban's nuclear power plant. They measured leak rate as a function of the inlet pressure (pressure at the outer diameter). Two sets of data were presented, each belonging to a different reactor coolant pump feeding the same nuclear reactor. The predictions of the current TEHL model are compared against Galenne and Pierre-Danos' $\bar{\mu}$ high fidelity TEHL model, based on a fully coupled FEA analysis. Additionally, the predictions of the simplified EHL model were compared against Liao et al.'s isothermal, fluid-structure interaction model.

Both the EHL and TEHL models compare favorably with the experimental measurements. The TEHL model, even though it over-predicts the leak rate at

higher pressure, when compared against higher fidelity Galenne's model, captures the non-linear trend of the experiments better than Galenne's mode, which virtually follows a linear increase in leak rate as a function of pressure. The over-prediction of the current model at higher pressure can be attributed to possible turbulence effects, which are neglected in the present model. At lower pressures, the Reynolds numbers are of the order of a few hundreds. If the surfaces are assumed to be very smooth ($Ra < 100$ nm), in the absence of any turbulence triggers, it can be safely assumed that the flow within the gap is laminar. When pressures are higher, the Reynolds numbers can increase to values above 1000, especially near the inner diameter, and the flow might be in the laminar-turbulent transition regime. This onset of turbulent effects might reduce the load carrying capacity of the fluid and result in lower leak rates, an effect not captured in the present, laminar-flow only model.

Meanwhile, even though the EHL models make concessions in the level of physical action, by neglecting all thermal effects, they result in reasonable predictions. Both the current and Liao's model capture the non-linearity in the experimental data much better, but quantitatively seem to match only a fraction of the experimental data sets. Thus, if quicker solutions are desired, a user might use the faster EHL model as a qualitative guide to reduce the number of required simulations of the slower TEHL model.

7.3.4 Parametric Studies

Now that the model predictions have been validated, parametric studies were conducted to understand the effect of parameters that are difficult to study experimentally.

Shaft Speed

During start up of the RCP, two activities are in process. The pressure is increased to the operating range, and the shaft speed increases to normal running speed. Present models are capable of studying the effect of both of these parameters simultaneously. At all times, seal leak rate is the parameter of critical importance. In this study, the variation in leak rate is studied as a function of shaft speed for different pressure values. The results are shown in fig. 7.14.

It can be seen that the EHL model fails to capture any change in leak rate when speed increases. This is reasonable as in the EHL model, the speed only factors in the Reynolds equation and is used to calculate the hydrodynamic load carrying capacity. However, the hydrodynamic effects in this case are not significant as the velocity due to the shaft rotation is perpendicular to the direction of the flow. Moreover, there is no change in film thickness along the direction of rotation, meaning the hydrodynamic load carrying capacity is negligible. Thus, the entire load carrying capacity is provided through the hydrostatic effects of the fluid entering at a very high pressure.

In the TEHL model, on the other hand, higher shaft rotation speed results in higher viscous heat generation. We can see higher speed leading to higher leak rates, especially for higher pressures, where the “poiseuille” components of the velocity would also be higher, thus resulting in even higher viscous heat generation (fig. 7.15). At higher velocities, higher viscous heat generation leads to decrease in fluid viscosity, thus making the fluid to flow easily leading to higher leak rate. However, higher heat generation also leads to more thermo-elastic deformation in the solids, thus reducing the gap for the fluid to flow through. These two conflicting

effects become more prominent at higher pressures, where a maximum leak rate can be clearly observed around the speed of 100 rad/s. Figure 7.16 shows the difference in behavior at low and high pressure gradients.

Face plate taper angles

The cross sectional geometry of the face plates governs the flow of the lubricant within the gap. Typical RCP seal face plates have two tapers, a minor taper closer to the inner diameter, and a major taper closer to the outer diameter. As can be seen in fig. 7.17, a larger taper angle should result in an overall thicker fluid film, possibly leading to a higher leak rate. The effect of varying the minor taper angle, keeping the major taper constant has been studied in this section.

Figure 7.18 shows the variation in leak rate during the pressurization process for various minor taper angles. For different minor taper angles, the EHL model follows similar behavior of decreasing slope with increasing pressure, with the leak rate approaching a steady state value above about 2000 PSI. Moreover, the leak rates are higher for higher taper angles. This is reasonable, as for smaller taper angles, the fluid sees a smaller gap at R_i which leads to a lower leak rate.

On the other hand, the TEHL model (fig. 7.18b) exhibits a near-linear increase of leak rate with increasing pressure. This is consistent with the observation made earlier in fig. 7.13. Another interesting observation is the fact that the curves for different taper angles seem to become parallel for pressures higher than about 1200 PSI. This shows that above 1200 PSI, the increase in the leak rate becomes independent of the minor taper angle. Or, the thermo-elastic deformations near the inner-diameter cancel out the increase in film thickness for higher taper angles, thus making the film near the inner diameter a function of the film thickness at R_i only.

7.3.5 Model Limitations

Once again, the presented PAML+ model for mechanical seals has several limitations. The model neglects the effect of the entire stator and rotor support assembly. Meaning, the model is heavily limited in its capacity to study the effect of the surroundings on the seal performance. Similar to the other applications, the PAML+ model for seals is solving for the quasi-steady state operation. Which means that the model is incapable of studying the effect of dynamic loads such as shaft vibrations, or ambient noise. Another significant limitation of the model is that it is restricted to axisymmetric scenarios. As a result, the model is unable to predict potentially hazardous situations such as misalignment between the faceplates, or the “beaching” phenomenon, where foreign particles are deposited on a section of the faceplate. Lastly, the model uses the annular plate theory for faceplate deformation. This applies further limitations on the modes of deformation that the faceplates can experience, forcing the “bending” of the faceplates to be the dominant mode of deformation.

7.4 Conclusion

A new thermoelastic hydrodynamic lubrication model has been developed for the reactor coolant pump’s first seal. The model integrated the effects of mechanical deformation through theory of plates, thermo-elastic deformation through FEA based influence coefficients, with fluid flow modeled through Reynolds equation and thermal transport modeled through thin film energy equation.

The proposed framework was then compared against experimental measurements

available in the literature. Temperature and pressure variation along the mean film thickness was compared against the predictions made by the TEHL model presented by [131], with a good match. The temperature distribution within the fluid film was also favorably compared against the TEHL model presented by [130, 132]. Lastly, the leak rate predictions made by the EHL and TEHL models were contrasted against comparable models from Liao et al [128] and Galenne and Pierre-Daons [131] respectively.

The model was then used to analyze the effects of thermal and mechanical deformation, by studying the influence of different operating parameters on leak rate while the system was pressurized from ambient to operating conditions. While varying shaft rotation speed the TEHL model showed higher leak rates than the EHL model. Also, in the TEHL model, the leak rates showed a non-monotonic behavior upon increasing shaft speed, with a maximum leak rate at about 100 rad/s (950 RPM). While increasing the taper angle, the TEHL model exhibited a near-linear behavior as opposed to an asymptotic behavior exhibited by the EHL model. Moreover, the TEHL model showed that the increase in leak rate, while increasing pressure, was independent of the minor taper angle for pressures higher than 1200 PSI.

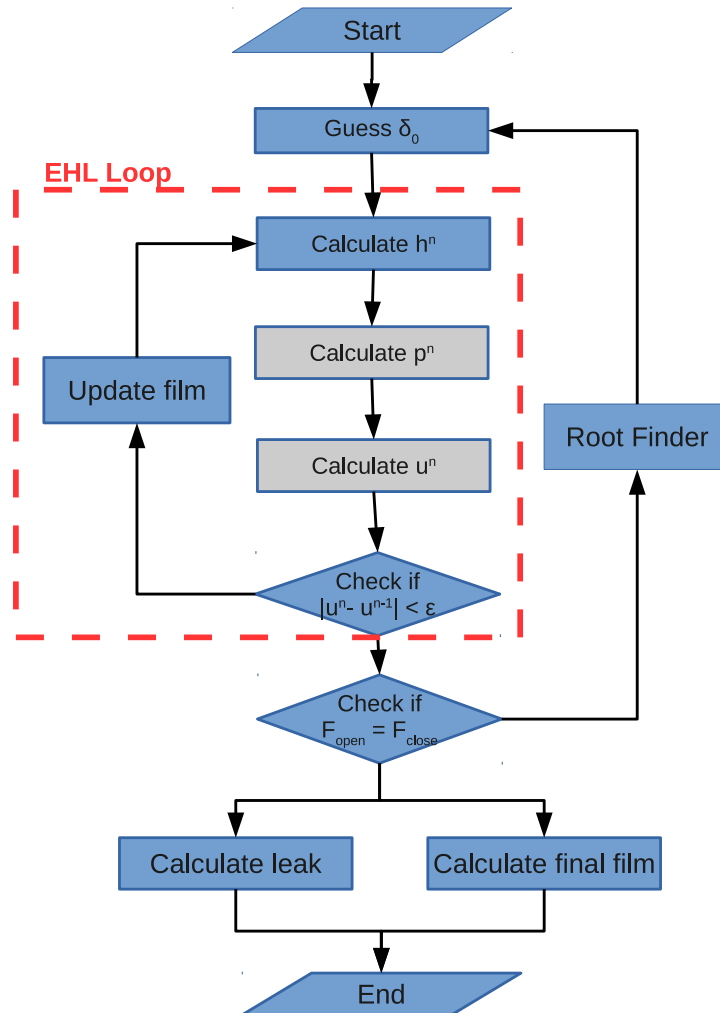


Figure 7.6: The flowchart for the EHL model. Note the inner “EHL loop” that ensures consistency between the fluid pressure and face plate mechanical deformation

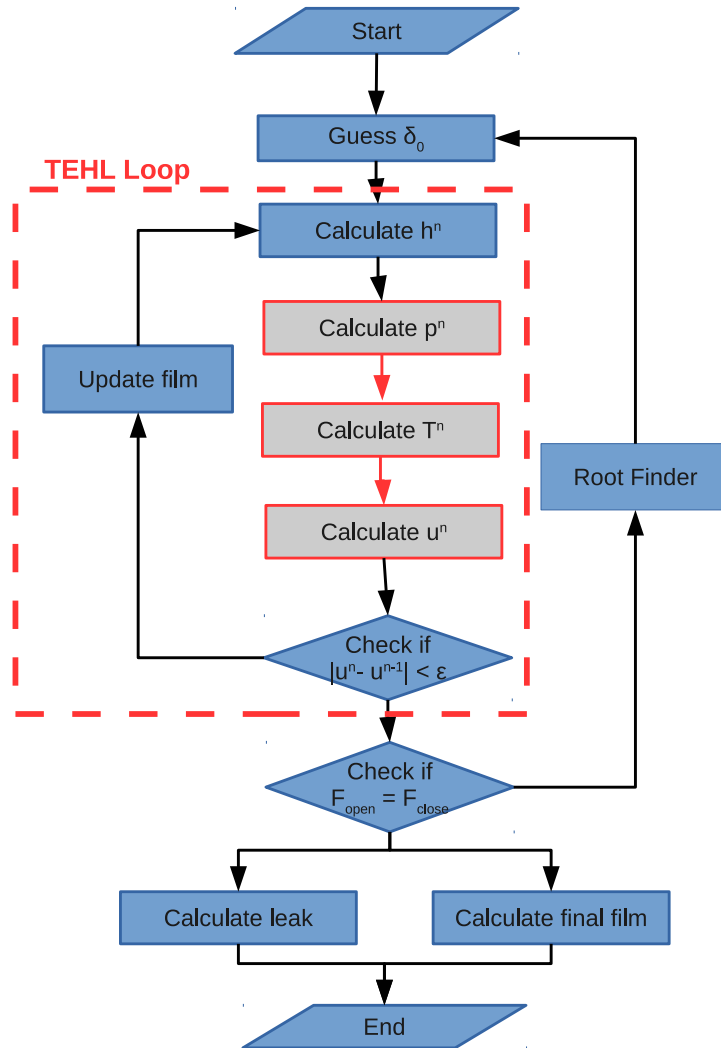


Figure 7.7: The flowchart for the TEHL model. Even though the inner TEHL loop is shown here as a simple three step process, it is collection of several complex, coupled steps. See fig. 7.8 for the detailed TEHL loop

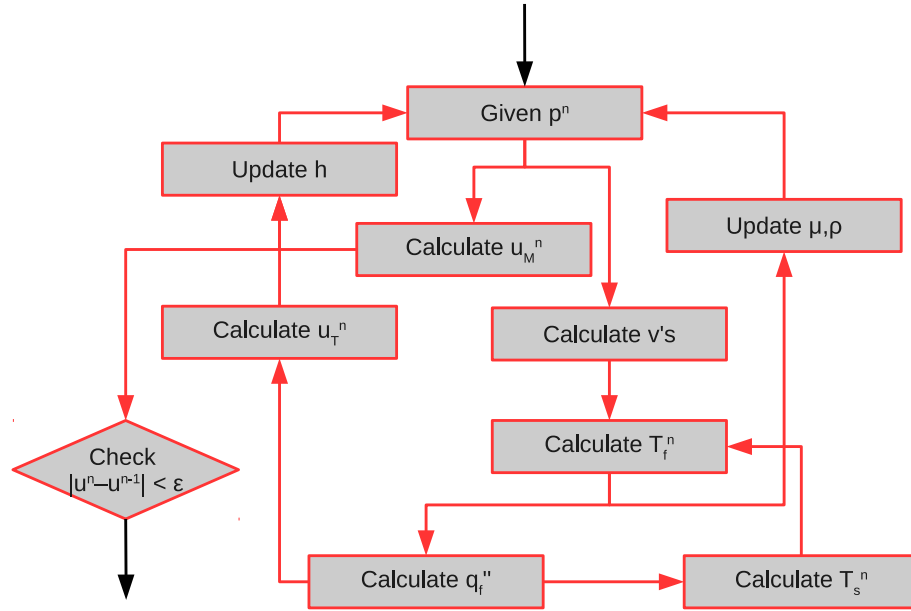


Figure 7.8: The TEHL loop that ensures consistency between the fluid pressure, the fluid temperature, solid temperature, and the face plate thermo-mechanical deformations

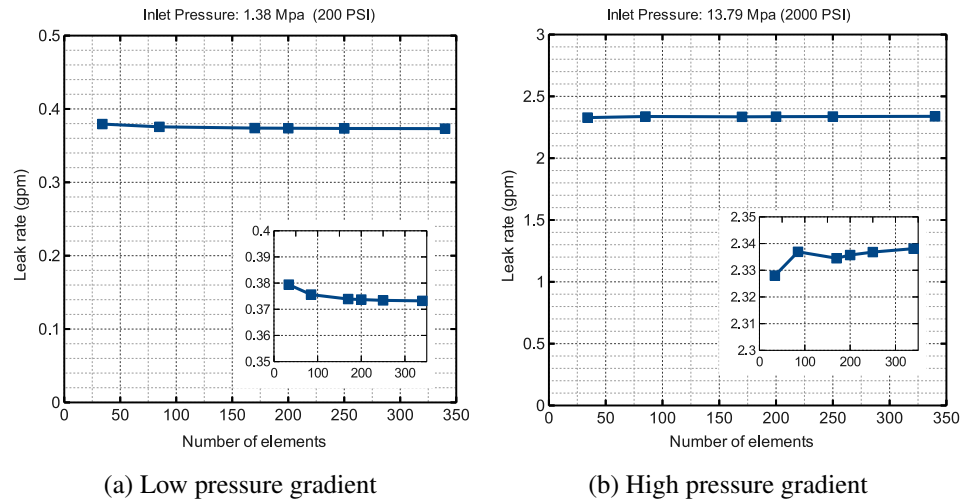


Figure 7.9: Leak rate as a function of grid size for low and high pressure gradients with inlet pressures of (a) 200 PSI, and (b) 2000 PSI, respectively.

Inset: Zoomed-in data

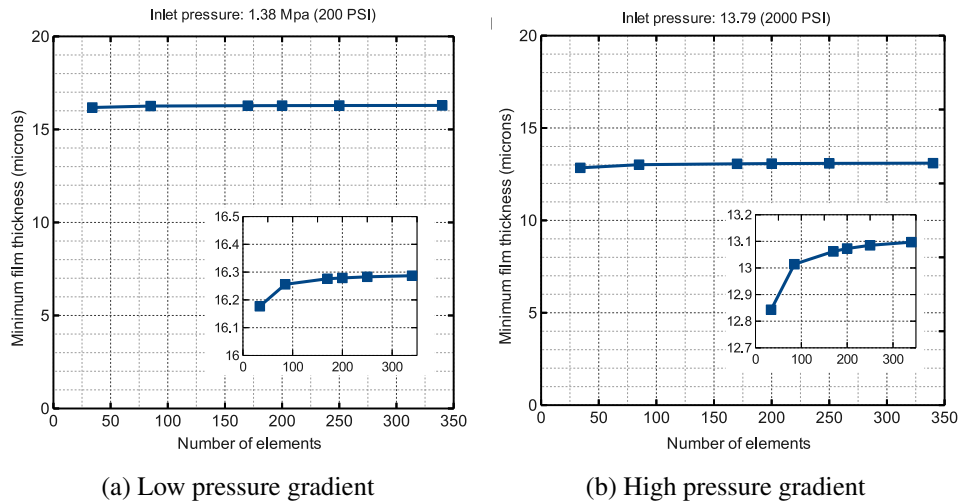


Figure 7.10: Minimum film thickness as a function of grid size for low and high pressure gradients with inlet pressures of (a) 200 PSI, and (b) 2000 PSI, respectively.
Inset: Zoomed-in data

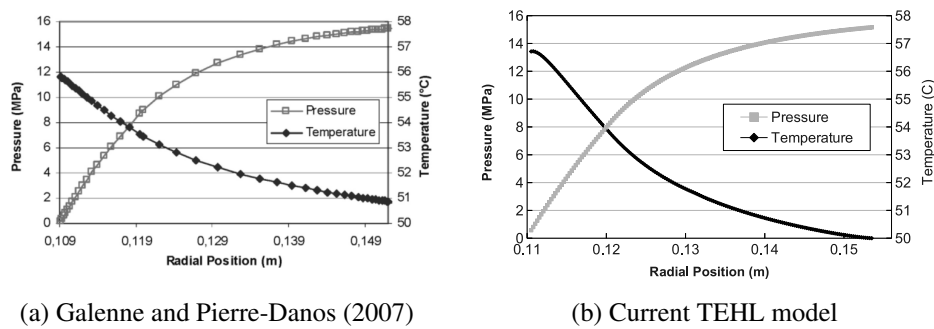
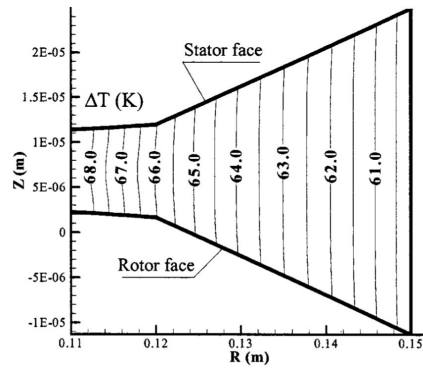
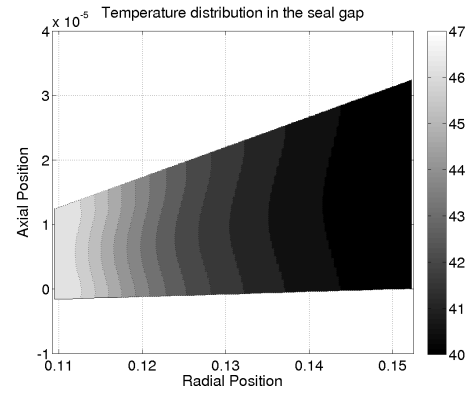


Figure 7.11: Pressure and temperature along the mean film thickness as predicted by two models

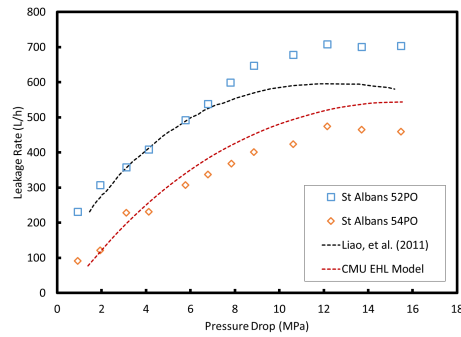


(a) Brunetiere et al. (2003)

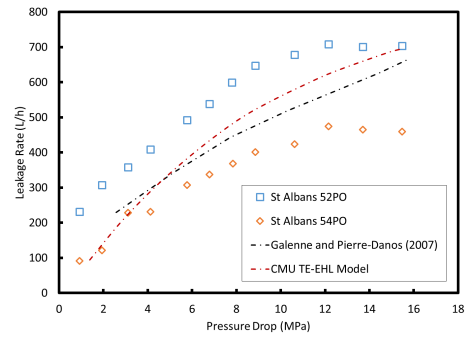


(b) Current TEHL model

Figure 7.12: Temperature distribution plotted over the fluid film geometry as predicted by two models

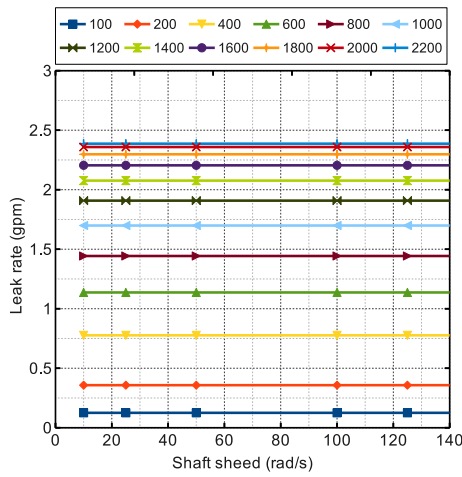


(a) EHL model comparison against Liao et al. (2011)

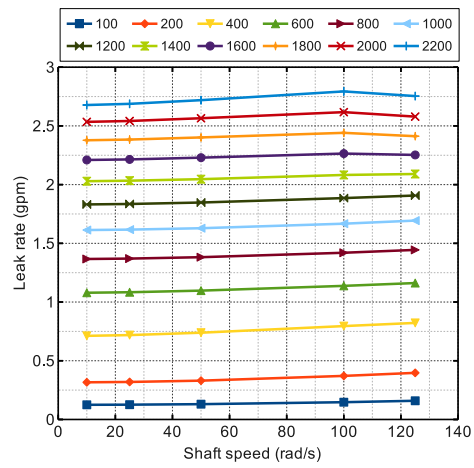


(b) TEHL model comparison against Galenne and Pierre-Danos (2007)

Figure 7.13: Leak rate as a function of inlet pressure (at OD) compared against other models and field data from Galenne and Pierre-Danos $\bar{\mu}_0$, measured at St. Albans power plant

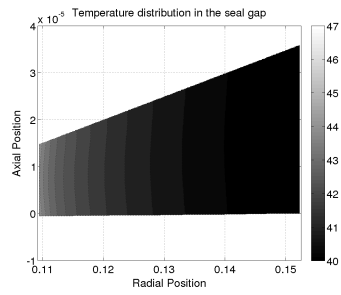


(a) EHL model

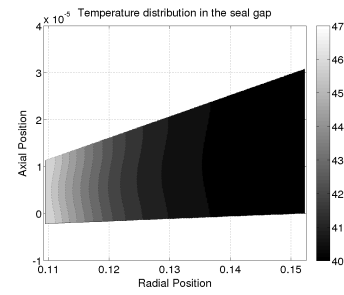


(b) TEHL model

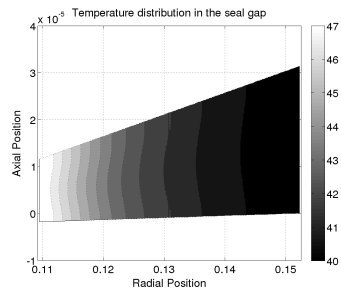
Figure 7.14: Leak rate as a function of shaft speed for several inlet pressures.
Outlet pressure fixed at 50 PSI



(a) Shaft speed = 10 rad/s
Inlet pressure = 200 PSI



(b) Shaft speed = 10 rad/s
Inlet pressure = 2000 PSI



(c) Shaft speed = 125 rad/s
Inlet pressure = 2000 PSI

Figure 7.15: Temperature distribution within the fluid film for different shaft speeds and inlet pressures. Increase in viscous heat generation can be clearly seen as pressure gradients and speed increase

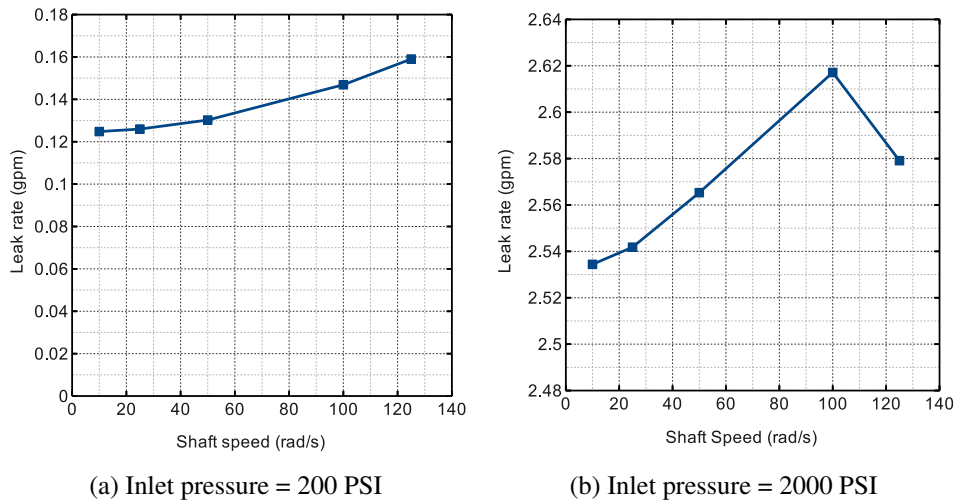


Figure 7.16: Leak rate as a function of shaft rotation speed for two different inlet pressures. Outlet pressure fixed at 50 PSI.

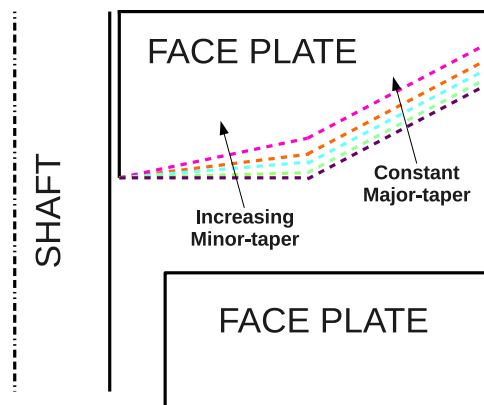


Figure 7.17: The variation in minor taper angle while keeping the major taper angle constant

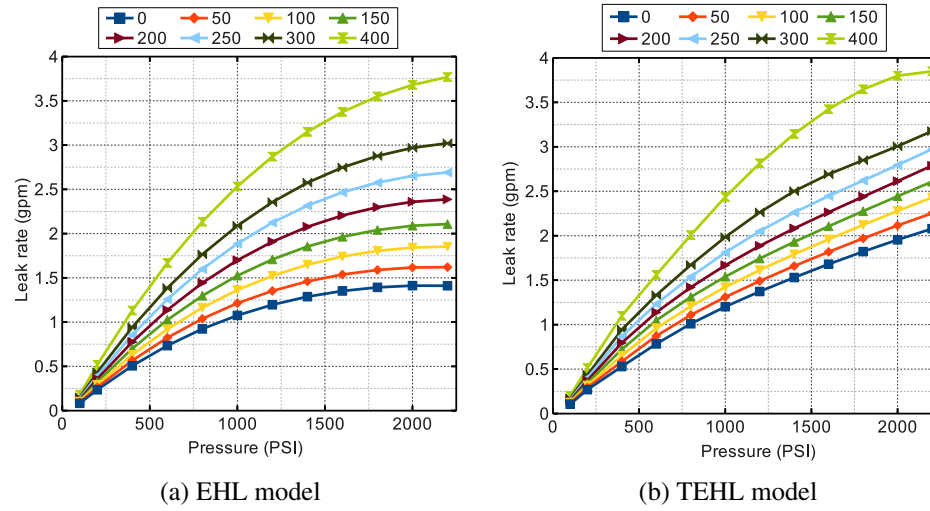


Figure 7.18: Leak rate as a function of inlet pressure for different values of minor taper angles (in μrad). For higher pressure gradients TEHL model demonstrates near linear behavior with pressure, similar to fig. 7.13. Major taper: $600 \mu\text{rad}$, outlet pressure: 50 PSI

Part III

Discussion

Chapter 8

Conclusion

The tribological behavior of any system is represented by wear and friction at the interface. Three distinct regimes of lubrication can be used to interpret the frictional response under given loading and motion conditions. It is common for industrial applications to proceed through multiple lubrication regimes over the course of their operation. As a result, a generalized modeling framework that can seamlessly traverse these different lubrication regimes is desired.

However, such models that can simulate all three lubrication regimes– boundary lubrication, hydrodynamic lubrication and mixed lubrication – are rare in the literature. Moreover, the models that do exist, either simulate simpler geometry and loading conditions than desired, or make over-simplifications regarding their physical interactions. In both of these scenarios, even though they achieve the capability to transition through different regimes, they lose their ability to serve as a broad utility for modeling tribosystems. The purpose of this work is to fill this gap and present a unified, widely applicable, industrial scale tribological modeling framework that does not sacrifice accuracy or computational efficiency.

The Particle Augmented Mixed Lubrication Plus (PAML+) modeling approach has been presented. It couples the fluid and structural behavior of any tribosystem. General steps involved while setting up a new application were outlined. A walk-through of example cases of a journal bearing and an artificial hip joint was also given. Additional modes of physics can then be added on this robust, “barebones” mixed lubrication modeling framework. Most common physical add-ons are particle dynamics and wear mechanics. Four applications were studied, through their own, dedicated, incarnation of PAML+, to demonstrate the strength and generality of the modeling framework.

1. **Pin on disc Tribosystem:** Simulating lubricated pin-on-disc tests involves characterization of the fluid-solid and solid-solid interactions. This application demonstrated the model’s capability to traverse through the different lubrication regimes. Upon increasing velocity or decreasing load, the model predicted transition from boundary lubrication to hydrodynamic lubrication, through the mixed lubrication regime. Friction and wear were measured during the simulation and used to study the effect of surface texturing. The model showed that surface texturing reduces friction within the system, and results in lower material loss, than untextured samples. This matched with experimental observations.
2. **Chemical Mechanical Polishing:** CMP operates in mixed lubrication regime. The model captured the fluid-solid, solid-solid, particle and wear mechanics in the process. Material removal rates predicted by the model matched well with the experimental measurements, specifically when studied as a function of load and particle sizes. Average pressure predictions also matched well

with dynamic pressure measurements published in the literature. Parametric studies revealed higher wear with decrease in fluid viscosity. Also, higher particle size variation was shown to increase material removal.

3. **Artificial Hip Joints:** As opposed to natural hip joints that operate in hydrodynamic lubrication regime, artificial hip joints are known to operate in boundary or mixed lubrication regime. Again, the model captured the fluid-solid, solid-solid, and the particle and wear mechanics within the joint. Realistic load and motion conditions representative of human gait cycle were implemented, and a general approach to repeat the process with other conditions was presented. Wear predictions of the model matched well with established numerical models, and experimental measurements made on hip joint simulators. Just as in the Pin-on-Disk application, surface texturing was again shown to improve tribological performance and enhance lifetime of the joint. Textures reduced wear by generating more fluid load carrying capacity, while at the same time enabled debris trapping. Parametric studies on texture geometry, however, showed that not all texture designs improve performance. A tool such as “PAML+ for artificial hip joints” should be used to optimize the surface texture design for best results.
4. **Mechanical Seals:** Mechanical seals or face seals as they are commonly known, operate in hydrodynamic or elasto-hydrodynamic lubrication regime. The seals used in the reactor coolant pump in a nuclear power plant, operate in extreme conditions enduring extremely high pressure gradients. High shearing leads to significant viscous heat generation in the gap which, together with high pressure gradients, results in thermo-mechanical deformation of

the seal face plates. Over its entire spectrum of operating conditions, the seal is required to operate in “controlled leakage” condition with precise control on the leak rates of the fluid. The model was used to study the fluid leak rate as a function of pressure gradient, representing the pressurization of the seal at start up. Model predictions matched well with experimental measurements, and with higher fidelity models. Parametric studies showed that thermal effects significantly influence the behavior of the seals. Increase in shaft speeds and decrease in taper angles are shown to exacerbate these thermal effects.

Chapter 9

Impact and Future Work

9.1 Impact

Tribology is the science of friction, lubrication and wear, and is critical for long-lasting design of industrial components. The tribological behavior of lubricated contacts can be identified by three lubrication regimes: dry or boundary lubrication, full film or hydrodynamic lubrication, and mixed-lubrication regimes. Unfortunately, optimizing design through experimentation in tribology, like in any other field, is a slow and expensive process and computational modeling is the desired alternative. The primary objective of this work was to develop a unified tribological modeling approach which is then demonstrated and evaluated by being applied to several industrial applications.

The author believes that PAML+ will give researchers a platform to combine different modes of physics on top of the robust fluid-structure coupling built into the framework. This will further expand the capability of the framework to newer

applications. The applications presented in this work will serve as example cases for future expansions.

Apart from just serving as examples, the models built for the applications studied in this work will bring novel insight into the research involving these applications themselves. Detailed impact of the current work on the individual applications is discussed below.

1. **Pin On Disc Tribosystem:** The major contribution of this model would be in the field of novel material design. Once the primary material properties are characterized, the model will make it easier to study newer and expensive materials for their tribological performance. Current approach at studying novel materials involves exhaustive experimental evaluation, conducted over hundreds of samples. The model can also act as a guide to reduce the number of such experimental investigations. Coupled with a few more design tools, it would provide a DFM-like (Design For Manufacturability) framework to allow designing of materials for desired frictional performance.
2. **Chemical Mechanical Polishing:** At its current state, the model: “PAML+ for CMP” can be used to study the impact of different polish parameters on the within wafer non-uniform material removal. Such parameters may include polishing load, platen speed, pad material, pad roughness etc. Additionally, for the first time, a model can be used to guide the design of polishing equipment by studying geometrical properties such as the pad diameter, pad-wafer axial separation, wafer carrier size etc. Never before has a single model captured the interplay of such a large range of parameters that influence the

polishing efficiency. The model can also be used to design consumables by studying the abrasive particle sizes distribution, slurry rheology, thermal performance etc. Further, the model can be expanded to study industrial scale polishing systems (see Appendix for an example).

3. **Artificial Hip Joint:** The PAML+ framework has, potentially, the highest impact in this application. The tool allows the study of the effect of newer parameters on tribological performance of the joints, similar to the other applications. However, for the first time, a computational tool will introduce inputs specific to a patient in the study of tribological performance of joint prostheses. This will allow the possibility of patient-specific, mass customization of artificial hip joints, each designed to its patients physiological characteristics and lifestyle. Coupled with an advanced fabrication process, such as Additive Manufacturing (AM) this can allow the next generation of artificial joints to outlive the patients.
4. **Mechanical Seals:** The model will allow real-time monitoring of safe operation. The model can take the upstream conditions as input and predict, in real time, the emergence of anomalous behavior. This would be strong step forward in preventing catastrophic failures such as the one in Fukushima Nuclear Reactor (Japan) from happening again. Moreover, similar to other applications, this model will also allow designing of newer components by accounting for effects that were difficult to study in the past. The model can also allow preliminary investigations into radical design changes, such as textured seals. Lastly, at its current state, the model also has the potential to study other tribosystems with similar a geometry, such as hydrostatic

bearings, thrust bearings etc.

9.2 Future Work

Several assumptions were made while developing models for individual applications. In the future, depending on the problem of interest, the modeling approach would be able to relax some of the constraints imposed by the applications studied so far. One such constraint was faster contact mechanics treatment, which has been treated with Winkler Elastic Foundation approach so far. Recent developments in the field of contact mechanics has made the discrete convolution with fast fourier transforms (DC-FFT) approach, which used to be resource intensive, much more computationally efficient. The next step should be to integrate the high resolution DC-FFT approach into the framework to allow the user to make the choice between high speed, high accuracy, and higher speed, lower accuracy. Unfortunately, another constraint that is still prominent with the DC-FFT approach is that it is only applicable to Cartesian coordinate systems. Spherical polar versions exist, but are not as robust as their Cartesian counterparts. If the migration to DC-FFT is to be made, the rest of the approach would also have to become coordinate system independent.

9.2.1 A Note of Humility from the Author to the Next Generation

While at first, it may appear that the PAML+ modeling framework has solved several complex tribological problems which by themselves could be core parts of a doctoral thesis, the author would like to add a note of encouragement to the next generation of tribology students.

There are several reasons why the PAML+ modeling approach should not be viewed as an over-reached attempt at solving many complicated tribology problems.

- 1 The focus of this work was on developing and assessing the modeling framework. Results presented throughout the different applications are, for the most part, preliminary, and rigorous testing and analysis would be important to prove the strength and flexibility of the framework.
- 2 The applications addressed through the current framework have several limitations as mentioned in sections: 5.3.5, 6.3.6 and 7.3.5. Based on these limitations, there is huge opportunity for improving the current incarnations of individual models for the applications studied in this thesis.
- 3 PAML+ was built to be a unified framework capable of seamlessly traversing different lubrication regimes (boundary lubrication, to mixed lubrication, to hydrodynamic lubrication regimes). However, due to the complexity of the load sharing mechanism, and changing modes of physics between dry and hydrodynamic lubrication regime, primarily in the form of solid deformation, it was difficult to obtain convergence in the Pin-on-disc application. Therefore, the model is not quite considered a unified model yet. It is recommended that the next student devise a better load-sharing mechanism, and improve the solid model that can accommodate both the contact based and fluid pressure based deformations.
- 4 Future students should look to leverage this modeling framework to focus on just one of the applications modeled in this work. Deeper, more extensive parametric studies are needed to explore the true power and capability of this

modeling framework, and to provide thorough understanding of the subject, fitting of an expert.

- 5 Following the first comment above, thorough experimental validation would greatly enhance the credibility of the predictions made by the model. Since the whole purpose of this modeling framework is to become a guiding tool for the industrial application, comparing the model against industry standards experiments is the only way to get the industry interested in the model.
- 6 Lastly, the unified “framework” which is essentially a collection of models dedicated to different applications, should evolve to become product of greater utility. The framework, which is currently a researcher’s model, should move towards becoming a “layman’s tool” that is capable of setting up the problem with relative ease. It would be slow, tedious process as industrial tribological problems are significantly different from each other, unlike, say a problem in just CFD. The biggest threshold would be to try and make the tool coordinate system independent. However, updating the contact mechanics framework to higher fidelity solutions might be the first step in that direction. Integrating this approach with an open source FEA solver can greatly simplify this transition from a “framework” to a “tool”.

Part IV

Supporting Material

Appendices

Appendix A

Industrial Scale Chemical Mechanical Polishing

Note: The model described in this chapter has been filed as an intellectual property by Carnegie Mellon University (CMU). Any for-profit use of the modeling approach described herein requires contacting the CMU Center for Technology Transfer and Enterprise Creation (CTTEC)

A.1 Abstract

Chemical mechanical polishing is an integral part of the electronics fabrication process. Lab scale experimentation and corresponding modeling studies have shed invaluable insight into the mechanism of CMP. Several models have been successful at predicting the interfacial fluid pressure, and overall MRR incurred in a benchtop polishing operation. However, the load and motion conditions are

completely different in an industrial scale polishing setup. Majority of the models that simulate benchtop polishing operation fail to account for the interactions that govern the behavior of a larger, multi-wafer polisher. A new multi-physics, industrial scale CMP model has been presented, based on the recently published wafer scale particle augmented mixed lubrication (PAML) modeling approach. Older models either ignored different modes of physics to accomplish wafer scale calculations, or remained in the feature scale to account for more physical interactions. Whereas the wafer-scale PAML approach allows faster computations without sacrificing accuracy, which makes it ideal for macroscale analyses. The present work, an extension of the wafer-scale PAML approach, is capable of capturing the interfacial phenomenon in an industrial scale polisher. Results for variation in the fluid pressure, contact stress and wear for different wafers have been presented.

A.2 Introduction

Chemical mechanical polishing has been a critical process for achieving surface planarization in electronics, and is commonly used as an intermediate fabrication step for devices such as integrated circuits [68], light emitting diodes [69, 70] and magnetic hard disk read/write heads [71]. CMP involves complex interaction between the workpiece, typically in the form of a wafer, an abrasive slurry, and a soft, conformal surface that results in nanoscale precision in material removal.

Even though CMP is extremely common in the industry, the tribological mechanism of the process is not completely understood. There have been numerous studies [3, 58, 61, 68, 69, 71, 73, 76, 81] trying to explain the mechanical and chemical

actions during CMP. Thanks to decades of research, the current generation of CMP engineers have managed to develop acceptable predictive capability for polishing performance. However, most of that understanding has been guided by numerical investigations, simulating a lab-scale polisher with simplified load and motion conditions. Research scale polishers include a simple pad with finite adjustments on its speed, a single stationary wafer carrier, and typically a finite range of load applications. Modeling studies conducted on such setups often, though rich in their investigation, are not focused on the yield or throughput of the polishing operation. But foundry manufacturing scale CMP, to reduce costs, requires larger volumes and higher throughput. Hence, studies conducted on the benchtop polishers are being unable to provide process engineers with actionable information for industrial scale machines which have multiple wafer polishing heads.

To guide researchers devising industrial polishing recipes for newer applications, computational models must be developed that can simulate the behavior at large length and time scales. Moreover, since the CMP process recipes in manufacturing-scale polishing are fine tuned to extreme levels of precision in consumables (pad and slurry selection) and operating conditions (load, motion and thermal conditions), a rigorous physics-based model must still be employed to account for the numerous operating and consumable variables. In this paper, a multi-physics model, based on the principle of wafer-scale particle augmented mixed lubrication (PAML) [62] is presented to simulate the behavior of an industrial scale, multi-wafer polisher.

A.3 Modeling Scheme

An industrial scale polisher has several wafer carriers mounted over the platen. Each wafer carrier, is then capable of polishing several wafers simultaneously. Figure A.1 shows a simplified schematic of the polishing setup thus obtained. Figure A.1b shows the orientation of a wafer carrier over a larger pad. Several wafers are mounted within each wafer carrier, in an arrangement shown in Fig. A.1a.

The modeling approach followed by Srivastava and Higgs [62] has been extended in this work to simulate the large, industrial scale, multi-wafer polisher. Similar to [62], the philosophy of the modeling scheme has two parts: determining the dynamic equilibrium orientation of the system, and calculating the material removal. As shown in Fig. A.1b, similar to a single wafer polisher, the wafer carrier is mounted on a gimble joint that is unable to provide moment reactions. Thus, the state of dynamic equilibrium is achieved when the net forces and moments acting on the wafer carrier, vanish. Due to apparent circular symmetry in the process, the net horizontal force (in X and Y directions), and vertical moment (in Z direction), are assumed negligible. Thus, for dynamic equilibrium, the only conditions required to be satisfied are $F_z = 0$, $M_x = 0$ and $M_y = 0$.

During operation, apart from the frictionless tangential sliding between the wafer and the wafer carrier, the two components would be in static equilibrium. Thus, it is assumed that the forces acting on the wafers are directly transferred over to the wafer carrier. The major forces acting on the wafer during CMP are the hydrodynamic pressure applied by the slurry, the contact pressure applied by the pad asperities,

the friction resulting from the contact pressure, and the external load applied on the wafer carrier. The slurry flow is assumed to be incompressible and Newtonian and the pad material is assumed to be linear-elastic and isotropic. Although there is frictional heat generation in the partial contact between the wafer and the pad which results in elevated pad, wafer and slurry temperatures, the analysis here is assumed to be isothermal. Increased temperature directly affects the behavior of the slurry by changing its properties (density and viscosity). The temperature rise also elevates the rate of chemical reaction, affecting the mechanical properties of the wafer and the pad as well. The combined effect of these modifications in the mechanical properties of the wafer, pad and slurry, in turn, influences the material removal rate. The isothermal assumption, thus, simplifies the analysis, making it more appropriate in the absence of chemical effects.

Based on the assumptions mentioned above, a comprehensive model is presented here that accounts for the effect of the slurry, solid - solid contact between the wafer and the pad, and wear due to the abrasive particles in the slurry. The following sections describe the major components of the model.

A.3.1 Fluid Modeling

The slurry has a very strong effect on the polishing performance. Some authors have even claimed that the chemical erosion is the dominant material removal mechanism in CMP and have hence focused their entire approach towards accurate prediction of the behavior of the slurry [75, 76]. The slurry also has several chemical additives that enhance its polishing performance. The additives adsorb and react with the surface of the wafer, altering its thermo-mechanical properties, and thus affecting

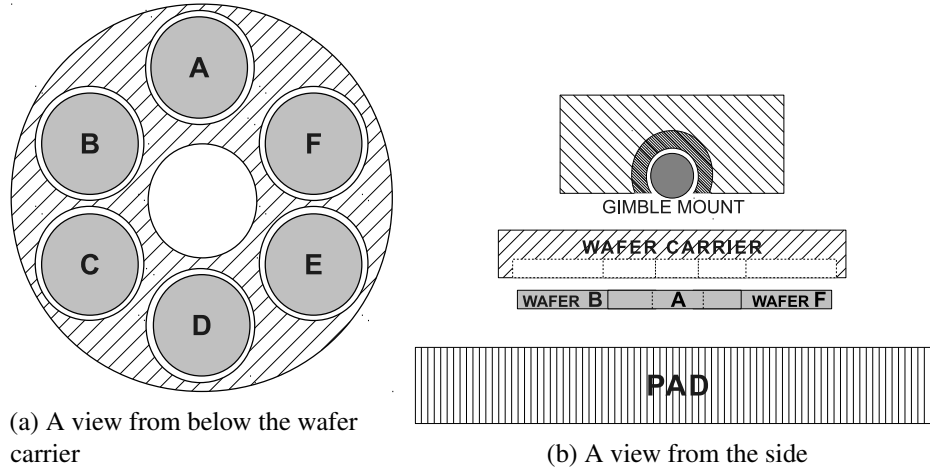


Figure A.1: A schematic showing the arrangements of the wafer carrier over the pad. Also shown is the arrangement of six wafers within the wafer carrier.

the material removal rate. However, for the purpose of this work, the analysis of the slurry has been restricted to its mechanical or hydrodynamic behavior only.

In the presented model, the hydrodynamic pressure generated in the wafer-pad interface plays an important role in determining the equilibrium orientation of the wafer carrier. Following the approach of [62], the Reynolds Equation has been solved to calculate the hydrodynamic pressure acting on the wafer surface. Due to the cylindrical-polar geometry of the interface, the cylindrical-polar form of Reynolds Equation (eq. (A.1)), given by Beschorner and Higgs [66] has been used in the current model. The industrial scale polishers also operate in the mixed lubrication regime. In the wafer-pad interface, the film thicknesses are small, and the flow can be assumed to be fully developed, laminar flow. The Reynolds equation has been shown to accurately capture the behavior in the case of CMP operation [75]. The slurry has been shown to exhibit slight shear thinning behavior which is typically

modeled as a power-law Newtonian plateau [136]. However, rheological studies have reported that the effects of shear thinning become significant at relatively high shear rates that are rarely encountered in a typical CMP operation [136, 137]. Based on these reports, the current work has assumed the slurry to exhibit Newtonian behavior. Even though the current analysis has neglected the effect of thermal transport, experimentally, temperature changes would affect the polishing performance. The viscosity decreases with increasing the slurry temperature leading to lesser magnitude of fluid pressure, eventually affecting the material removal rate. If the average fluid pressure under the wafer is largely negative, as is the case with rigid, rotating wafers [58, 138], this viscosity drop would decrease the material removal rate. However, if the wafers are flexible, causing a largely positive fluid pressure [139], a decrease in viscosity would lead to higher material removal rate. The reader is referred to the previous work of the authors [62] for some examples of evolution of material removal rate with changes in viscosity.

$$\begin{aligned} & \frac{1}{12\eta} \left[\frac{\partial}{\partial r} \left(rh^3 \frac{\partial p}{\partial r} \right) + \frac{\partial}{r \partial \theta} \left(h^3 \frac{\partial p}{\partial \theta} \right) \right] = rv_{r(w)} \frac{\partial h}{\partial r} - v_{\theta(w)} \frac{\partial h}{\partial \theta} \\ & + \frac{\partial}{\partial r} \left(\frac{v_{r(p)} + v_{r(w)}}{2} rh \right) + \frac{\partial}{\partial \theta} \left(\frac{v_{\theta(p)} + v_{\theta(w)}}{2} h \right) \end{aligned} \quad (\text{A.1})$$

Film Thickness

The primary quantity dictating the fluid pressure (p) in the Reynolds Equation (eq. (A.1)) is the film thickness 'h'. The film thickness in this model has been approximated as the separation between the smooth wafer surface, and the mean plane of the pad asperities. The individual contribution of the nominal clearance (δ_0), rolling angle (α) and pitching angle (β) have been superposed to give the

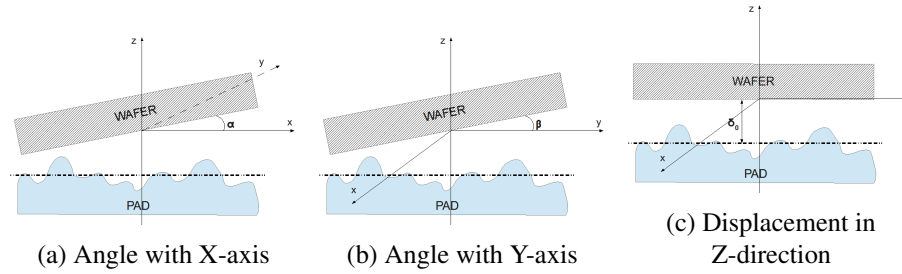


Figure A.2: Superposition of individual variables to calculate the film thickness

effective film thickness at a point (Fig. A.2). The resultant film thickness can be written as shown in (A.2).

$$h(r, \theta) = \delta_0 + r \sin \alpha \cos \theta + r \sin \beta \sin \theta \quad (\text{A.2})$$

Entraining Velocities

One of the key differences in an industrial scale polishing setup and a research scale single wafer polisher is the number of motion axes. Traditional benchtop, single wafer polishers only controlled the rotation of the pad, with the wafer carrier often kept stationary. Newer single wafer polishers now have the capability to control the rotation of both the pad and the wafer carrier. This is believed to reduce the non uniformity in the material removal across the wafer. The industrial wafer adds an additional level of complexity by allowing the wafer(s) to rotate with respect to the carrier. In some polishers, the wafers are attached to a ‘wafer mount’ and prescribed a rotational velocity. More commonly, the wafers are freely mounted on the carriers which allows them to “roll” due to the pad and slurry friction, which

again results in relative sliding between the wafer and the wafer carrier. Thus, there are three independent motions contributing to the polishing process. Figure A.3 shows the three angular velocities, enacting on the three components: the pad, the wafer carrier, and one of several wafers mounted on the wafer carrier.

The velocities have been calculated with the wafer carrier's center as the origin. Similar to a single wafer polisher, the pad and the wafer carrier have prescribed velocities. For simplicity, it was assumed that the wafers are spinning at a constant angular velocity as well, which remains constant with time.

The velocity of any point on the wafer, with respect to the ground, would be a vector sum of the velocity of the carrier, and the velocity of the wafer with respect to the wafer carrier. The net velocity of a point (r, θ) on the wafer carrier is given as (A.3). The pad velocity at the same point can be given as (A.4). Figure A.3 shows the different rotations, and their influence on the velocities.

$$v_{r(w)} = \Omega_w (r - r_{wc} \cos(\theta_{wc} - \theta)) + \Omega_c r \quad (\text{A.3a})$$

$$v_{\theta(w)} = \Omega_w r_{wc} \sin(\theta_{wc} - \theta) \quad (\text{A.3b})$$

$$v_{r(p)} = r_{cp} \sin \theta \Omega_p \quad (\text{A.4a})$$

$$v_{\theta(p)} = (r + r_{cp} \cos \theta) \Omega_p \quad (\text{A.4b})$$

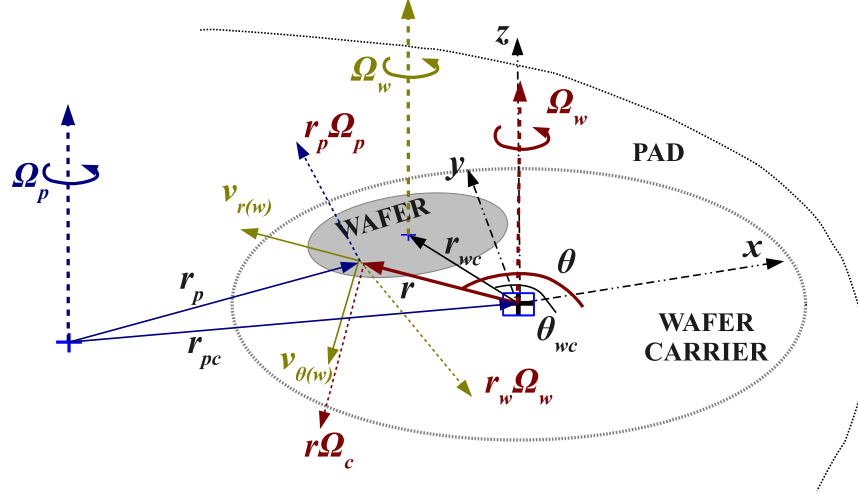


Figure A.3: Velocities in the wafer carrier coordinate system (only 1 of 6 wafers shown). Radial ($v_{r(w)}$) and tangential ($v_{\theta(w)}$) velocities of any point on the wafer (having coordinates (r, θ) with the center of the wafer carrier as the origin), is the vector sum of the wafer rotation ($r_w \Omega_w$), and the wafer carrier rotation ($r \Omega_c$)

The Reynolds equation (A.1), has been solved numerically through finite differencing over a two-dimensional $(r - \theta)$ grid. In the radial direction, Dirichlet boundary conditions ($atr = R_c; p = p(\theta) = 0$) has been used for the pressure. Tangential boundaries are naturally periodic.

A.3.2 Wafer-Pad Contact

During CMP, the applied polishing load is shared by the fluid pressure and the contact stress generated during the solid-solid contact between a rough pad and a (relatively) smooth wafer. Typically, the pad is made of a soft polymeric material placed on top of a rigid metallic platen. The wafer typically is a metallic, metalloid or ceramic material, and is much tougher than the polymeric pad. Thus, the solid-solid contact between the wafer and the pad can be modeled through

a Winkler Elastic Foundation [67] which approximates the softer material as a mattress, constructed by assembling a set of parallel springs. In this case, each spring represents a collection of, or a single asperity, occupying a rectangular area, and representing the average height of that area. It is assumed that these springs deform vertically, without influencing their neighbors. This provides a relationship (eq.(A.5)) between the stress and normal deflection for each spring, as has been described by Johnson [67]

$$\sigma(x,y) = K \frac{u(x,y)}{\tau} \quad (\text{A.5})$$

where, σ is the contact pressure, τ is the initial height of the foundation, and u is the deformation at the surface. The following assumptions were made to determine the proportionality constant:

- Tangential deflection of the asperities is neglected
- The effect of the tangential loads on the normal deflection is neglected

With the above assumptions, the equations of elasticity for the pad can be condensed to eq. (A.6)

$$\sigma(x,y) = \frac{E_{pad}(1-\nu_{pad})}{(1-2\nu_{pad})(1+\nu_{pad})} \frac{u(x,y)}{\tau} \quad (\text{A.6})$$

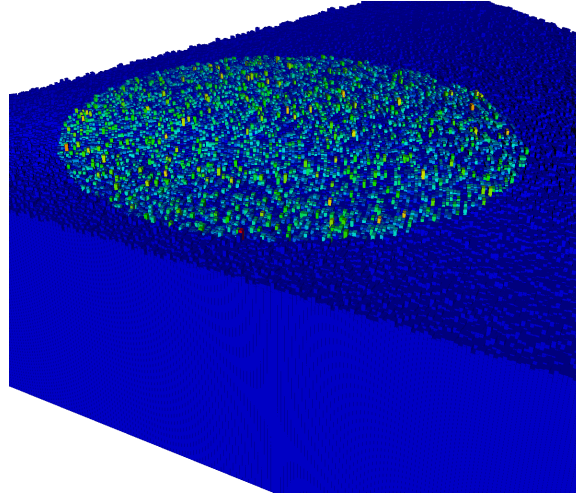


Figure A.4: A sample surface topography of a section of the pad. The colours represent contact stress during a typical wafer-pad contact situation (see Sec. A.4.2) for more details

This expression explicitly relates the normal stress $\sigma(x, y)$ to the normal deflection $u(x, y)$ of an asperity. As a result, the calculation of contact pressure can be obtained through $O(N)$ operations, which is critical to maintaining the speed and memory efficiency of PAML-lite. Also, it organically enables the solution of a rough contact problem. Figure A.4 gives an idea of the roughness of the pad.

A.3.3 Equilibrium Orientation

The fluid and contact pressure fields are used to formulate three equations in three independent variables mentioned earlier, the nominal clearance (δ_0), rolling angle (α) and pitching angle (β). The three equations correspond to the equilibrium conditions of no normal force ($F_z = 0$), and no tangential moments ($M_x = 0, M_y = 0$)

on the wafer. The equations are non-linear, implicit equations and, hence an analytical solution is not possible. The root finding approach followed in [62] has been followed to obtain the solution of this set of 3 simultaneous equations.

A.3.4 Wear

Abrasive wear has been widely accepted as the predominant wear mechanism during CMP. Following the definition of abrasive wear, a "wafer-wear" event only occurs when an abrasive particle indents into the wafer surface, due to force applied by the pad asperity. The method proposed by Luo and Dornfeld [73, 79], and outlined in [62] has been followed here to calculate material removal for each wafer.

A.4 Results

The Reynolds Equation was solved numerically using the wafer center as the origin. The entire region under the wafer carrier was discretized into a polar rectangular grid. The pad was independently discretized into another polar grid with the center of the pad as the origin. For calculating the contact stress, a rough pad surface was used with a mean height and average roughness specified in Table A.1. The pad was assumed to be a Rodel IC1000, the wafer was assumed to be a blanket Cu surface. The slurry was assumed to be an aqueous silica suspension.

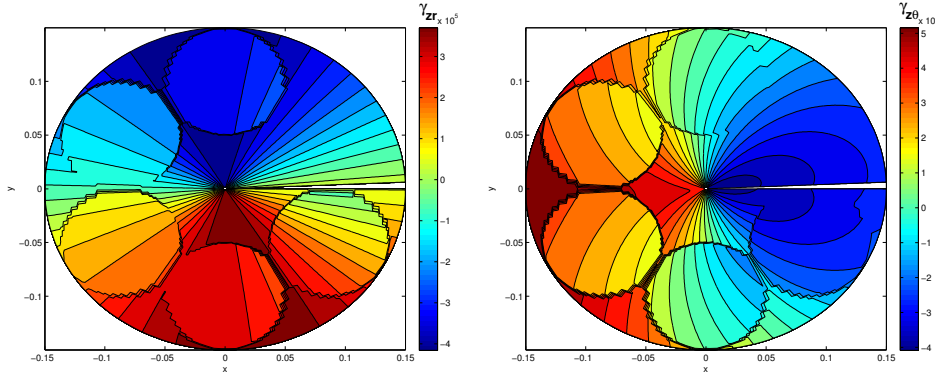
A.4.1 Shear Rates

As in any other application of the mixed lubrication regime, in CMP, the fluid entrained between the wafer and the pad surfaces endures extreme levels of shearing. In a typical benchtop setup, as the wafer is stationary, the shear rate is proportional

Table A.1: Model Parameters

Pad Properties	
Model Simulated	IC 1000
Elastic Modulus (Bulk)	12 MPa
Elastic Modulus (Tip)	300 MPa
Poisson's Ratio	0.4
Hardness	5.0 MPa
Asperity Distribution	Gaussian
Thickness	1.3 mm
Roughness	5 μm
Wafer Properties	
Elastic Modulus	110 GPa
Poisson's Ratio	0.16
Hardness	2.0 GPa
Slurry Properties	
Solvent	Water
Solvent density	1000 kg/m ³
Abrasives	SiO ₂
Abrasive Density	2000 kg/m ³
Abrasive Size Distribution	Gaussian
Mean Abrasive Diameter	150 nm
Standard Deviation of Abrasive Diameter	70 nm

to the velocity of the pad. In some of the advanced research scale polishers, the shear rate becomes more complex when the wafer, mounted on a movable carrier, starts rotating. However, in an industrial scale polisher, since there are three independent rotating components, the pad, the wafer carrier and the wafer themselves, the shearing of the fluid is extremely complex. A simple indicator of this shearing can be expressed as a nominal shear rate, which is the difference between the velocities of the top and bottom surfaces, over the local film thickness, eq (A.7). This variation in the shear rate under the wafer carrier is shown in Fig. A.5. It can be observed that there is a large non-uniformity in shearing across different wafers,



(a) Shear rate within the interface along the radial direction (γ_{zr}) (b) Shear rate within the interface along the tangential direction ($\gamma_{z\theta}$)

Figure A.5: Fluid shear rate along the radial and tangential directions, at time step=0. This represents the complexity in the motion of the fluid within the interface, due to a combination of three rotations: of the pad, of the wafer carrier and of the individual wafers

and even within single wafers. This variation in turn, affects the generated fluid pressure within the gap (see sec. A.4.3). The variation in the fluid pressure then results in net moments on the wafer carrier eventually generating non uniformity in wear. However, since the wafers themselves are rotating, and the shear rate remains virtually fixed throughout the polish, different sections of the wafer should end up wearing similarly, thus producing a reasonably smooth surface.

$$\gamma_{rz}(\dot{r}, \theta) = \frac{v_{r(w)}(r, \theta) - v_{r(p)}(r, \theta)}{h(r, \theta)} \quad (\text{A.7a})$$

$$\gamma_{r\theta}(\dot{r}, \theta) = \frac{v_{\theta(w)}(r, \theta) - v_{\theta(p)}(r, \theta)}{h(r, \theta)} \quad (\text{A.7b})$$

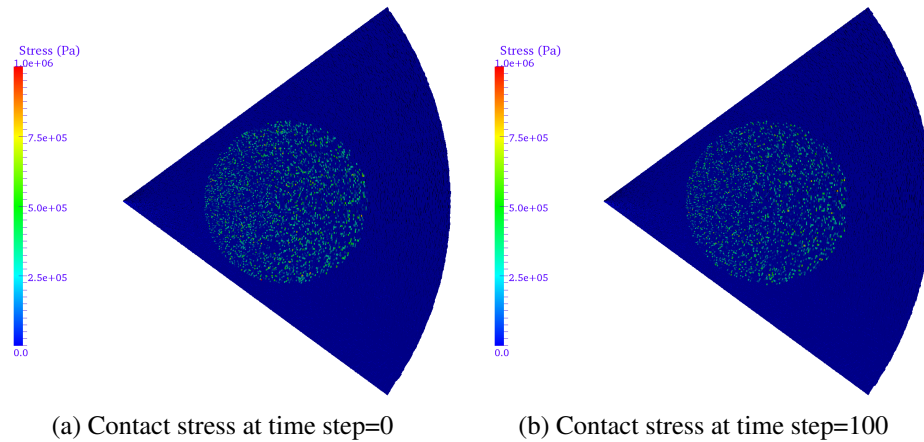


Figure A.6: Contact stress experienced by the asperities of the pad. At every time step, the contact stress and the fluid pressure, together, balance the applied polishing load.

A.4.2 Contact Stress

As the model is based on the hypothesis of the process occurring in the mixed lubrication regime, the solid-solid contact between the wafers and the pad changes with time. Naturally with a different pad asperity distribution, the contact stress experienced by points on the wafer also changes, which in turn results in changes in material being removed from the wafer surfaces. Figure A.6 shows the distribution of pad contact stresses at two instances.

A.4.3 Fluid Pressure

As mentioned in the previous section, the equilibrium orientation of the carrier, on the gimble mount (Fig. A.1b) changes with every time step. As a result, the film thickness also evolves with time, and depends strongly on the asperity distribution. This change in film thickness, in turn, affects the fluid pressure distribution under

wafer carrier. Figure A.7 shows the distribution of fluid pressure at two different time steps. It can be seen that the fluid pressure is higher at regions under the wafer, and drops as you move away from a wafer center. This means that the wafers themselves experience a positive fluid load carrying capacity, with the fluid resisting solid-solid contact. Another observation that can be made is that at time step = 0, the fluid pressure under the wafer carrier, outside the wafers, is largely negative, whereas it becomes almost entirely positive at time step = 100. Clearly, there can be significant difference in the net load being supported by the fluid pressure over time, which would lead to significantly different material removal during different stages in the polish.

A.4.4 Material Removal

The mechanism for material removal during CMP is proposed to be abrasive wear. Meaning, during the polishing process the abrasives being transported by the slurry get trapped between the wafer and the pad asperities. The trapped abrasives then slide across the wafer, being dragged by the pad, and result in “abrasive” material removal from the surface of the wafer. Since this abrasive wear mechanism is based on solid-solid contact, the volume of material removed depends heavily on the contact stress pressing the abrasive on the wafer. As shown in the previous section, the contact stress can differ significantly over different time steps, the volume of material removed can also differ significantly over the entire wafer-pad interface. Figure A.8 shows the variation in thicknesses of Cu layer left on the wafers. Lower thicknesses reflect higher wear from the wafer surface. Significant differences in material removed can be observed between different wafers. Even within each wafer, there is tremendous non uniformity in the material removal. Still some interesting

observations can be made. The Cu thicknesses go from almost uniformly at $20\mu m$, to being closer to $19\mu m$. Half of the wafer of the wafers appear to be forming a ‘family’ of similar roughness, i.e. having a similar distribution of thickness.

The variation of wafer wear with applied polishing load was also studied. Figure A.9 shows dependence of an average material removal rate with polishing load. Overall, the model exhibits Prestonian behavior with the average material removal rate, i.e. the MRR varies linearly with increasing load. However, the model gives a deterministic wear distribution over the wafer surface, with sections of the wafer wearing more or less than this average values. Contrary to the Preston’s equation [3] which only gives a ‘statistical’ average of the material removal over the entire wafer surface.

Since abrasive wear is the only mechanism for material removal, the model predicts almost no material removal at near zero pressures. When no external load is applied, there would be virtually no contact between the pad and any of the wafers. Moreover, the wafer carrier would be lifted far above, being parallel to the pad surface. This would result in a thick, uniform film thickness over the entire wafer carrier-pad interface, leading to almost no hydrodynamic pressure.

A.4.5 Parametric Study: Platen Speed

The model was then used to predict the variation in the material removal rate as a function of parameters that affect polishing. In most polishing tools, the two easiest to change parameters are the polishing load and rotational velocities. Since the load was already used in validation, the chosen parameters were the wafer carrier speed

and the platen speed. Figure A.10 shows the variation of the material removal rate as a function of the wafer carrier speeds, for several pad speeds. Overall, it can be seen that the slowest moving pad results in the highest MRR. Since the load carrying capacity (LCC), i.e. the ability of the fluid to support a given load, would be strongly affected by the angular velocities of the three components, this shows that the LCC of the fluid has a strong influence on the material removal rate. Also, it can be seen that for all values of pad speeds, the material removal rate reaches a maximum value at the carrier speed of 40 RPM, and then drops exponentially beyond that. Again, with increase in the speed of the carrier, the load carrying capacity of the fluid increases, thus reducing the net solid-solid contact and eventually reducing wear.

A.5 Conclusions

A new physics based numerical modeling approach towards simulating the behavior of industrial scale polishing has been presented. The present model expands the recent wafer-scale particle augmented mixed lubrication modeling approach [62] to an industrial scale polisher. The present model is capable of capturing fluid, solid-solid contact and wear behavior of several wafers simultaneously mounted on a single wafer carrier, while undergoing two independent rotary motions. A third rotation, in the pad, adds on to the shearing of the fluid in the interface and creates complex pressure distribution under the wafers. The material removal rate exhibits a near-linear behavior with applied polishing load. Also, the MRR is shown to be highest when the carrier is spinning at a speed of 40 RPM, irrespective of the pad speed. Upon increasing the carrier speed further, the MRR drops exponentially to

about 33% of the initial value when the speed is doubled to 80 RPM. The model is expected to serve as a tool for process engineers designing recipes for foundry manufacturing scale polishing setups.

Future work is aimed at identifying industry partners with the experimental data with which the new model can be explored as a predictive tool. Additionally, the model can be a useful tool for conducting exhaustive parametric studies for the effect of slurry properties (e.g., viscosity, particle concentration, particle hardness, etc.), pad properties (e.g., topography, roughness, texture, viscoelasticity, etc.), wafer properties (e.g., hardness, topography, roughness, and material heterogeneity or patterns for dishing/erosion) and machine operating parameters (e.g., rotation rates, carrier loads, gimbal degree of freedoms, etc.).

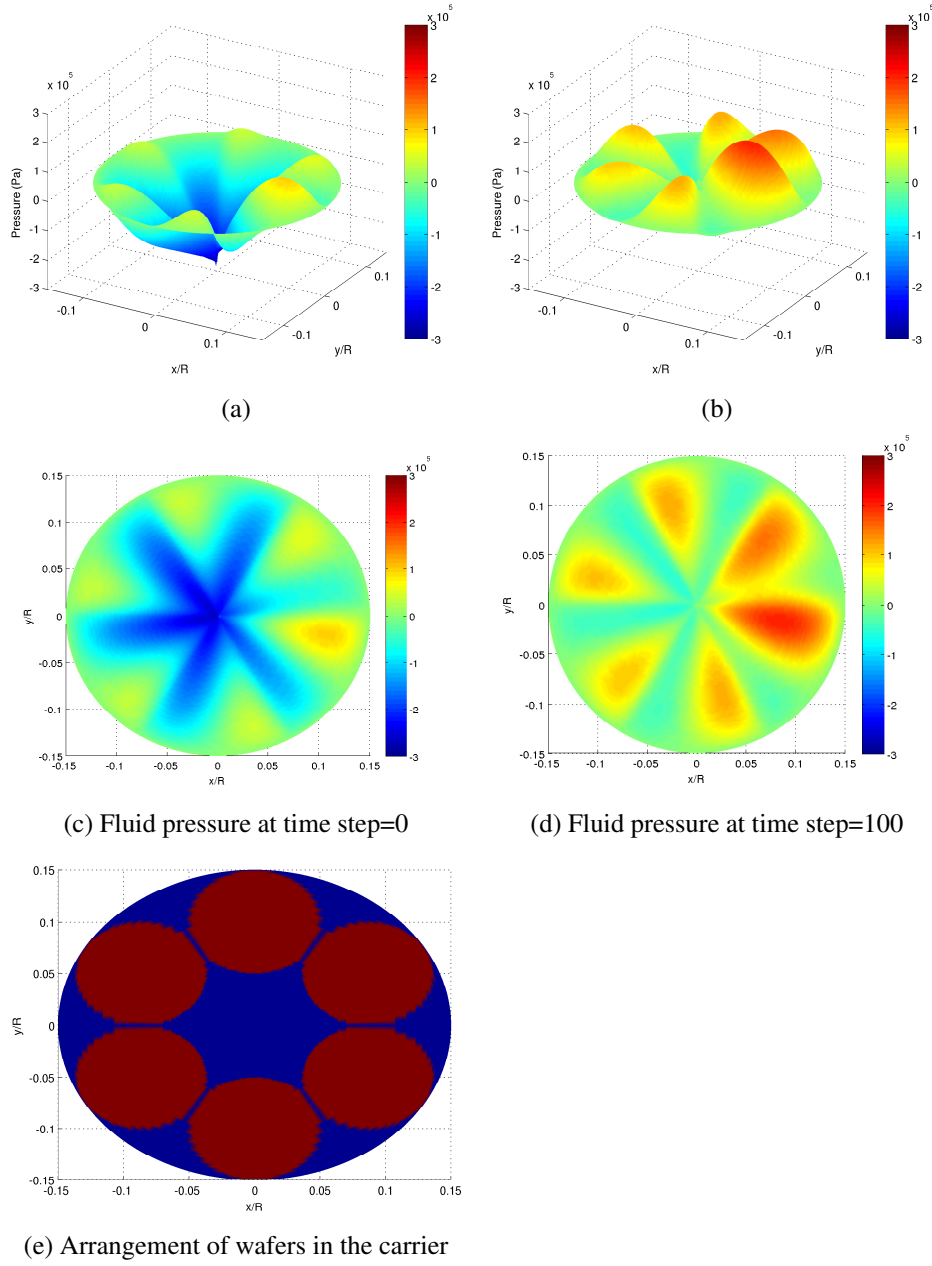


Figure A.7: Fluid pressure within the wafer-pad interface. (a), (b) show orthogonal views, and (c), (d) show contours of the pressure profile. The carrier is holding six wafers, as shown in (e)

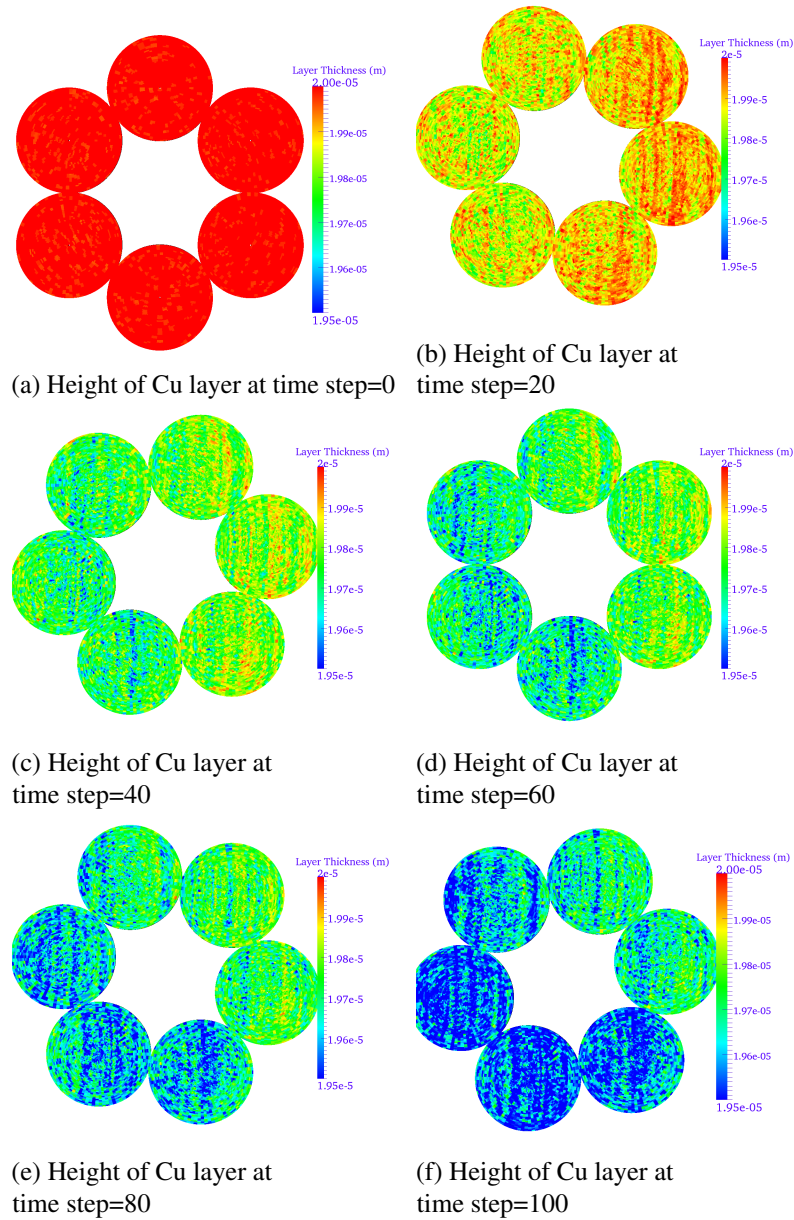


Figure A.8: Thickness of the Cu layer deposited on each of the wafers. Lower thickness reflects higher material removal. The positions of wafers changes with time due to the rotation of the wafer carrier. The position of each point on the surface of the wafer changes with respect to the corresponding wafer's center as well, due to the rotation of the wafer itself.

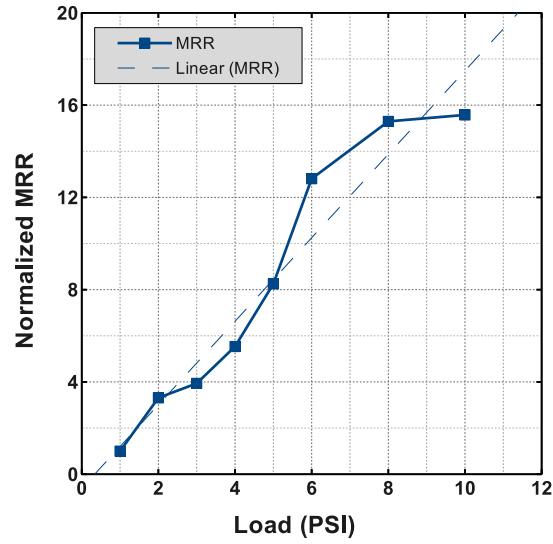


Figure A.9: Variation of material removal rate with applied polishing load. Linear behavior is observed, that matches well with Preston's equation [3]: which relates pressure (P), sliding velocity (v) with wear volume (ΔV), as: $\Delta V = kPV$

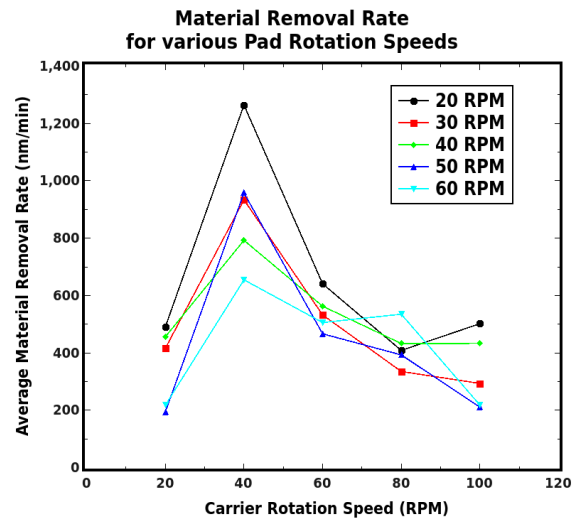


Figure A.10: Variation of material removal rate with the speed of rotation of the wafer carrier, for several platen speeds.

Appendix B

Thermal Effects in Chemical Mechanical Polishing

B.1 Abstract

Most chemical mechanical polishing (CMP) researchers assume that the polishing occurs in the mixed-lubrication regime, where the applied load on the wafer is supported by the hydrodynamic slurry pressure and the contact stress generated during the pad-wafer contact. Consequently, the particle augmented mixed lubrication (PAML) approach has been employed as an extremely high-fidelity asperity-scale mixed-lubrication CMP model in the past. Recently, a more computationally efficient PAML approach, PAML-lite, which considers the slurrys fluid and particle dynamics, the pad/wafer contact mechanics, and the resulting material removal, was introduced. The current work presents the PAML-lite framework with the isothermal assumption relaxed. As a result, wafer-scale interfacial temperatures during CMP can be predicted by considering asperity heating and dissipation of the

heat into the solid and fluid media in the sliding contact.

B.2 Introduction

There are several factors that affect the material removal procedure such as the chemical and / or mechanical effects of the contact pressure, relative velocity, types of pad and slurry, polishing temperature and other process conditions. Among these factors temperature is one of the most prevalent, still often overlooked factor that affects the material removal. White et al. [140] showed that the energy required to remove oxide and copper on a wafer is strongly correlated with the temperatures measured on the pad. Renteln and Ninh [141] showed that the activation energy of copper removal is on the order of 0.5–0.6 eV. This meant that 10⁰C increase in the pad temperature was sufficient to double the polishing rate. Pad temperature has also been used to monitor metal CMP process. Multiple authors have claimed that pad temperature can be used for endpoint detection. Hocheng and Huang [142] presented a list of patents that used thermal methods to monitor CMP process.

There have been multiple, somewhat similar explanations for the heat addition to the wafer-slurry-pad tribosystem. White et al. have claimed that the temperatures measured on the surface of the pad are a function of frictional force, relative velocity and polishing time. According to Oh et al. [143] the mechanical abrasion by the abrasive particles causes friction that generates frictional heat on the contacting interfacial area, and this heat plays a key role in accelerating the chemical reactions for material removal.

In this paper, a novel multiphysics framework has been introduced that can be used to model the thermal interactions between the wafer, pad and the slurry. The model accounts for majority of the physics affecting the CMP process: the hydrodynamic pressure generated by the slurry, stresses generated due to solid-solid contact, material removal by abrasives wearing down the surface, and heat generation at the wafer-pad interface due to friction. In the following sections, firstly the overall methodology of the model has been introduced. Then specific details about the thermal model have been discussed. Some of the possible outputs of the model have been discussed in the results. A parametric study that displays the predictive capability of the model was conducted. Predictive studies like these can be used to design better polishing processes in cases where experimental studies are cumbersome and expensive.

B.3 Modeling Scheme

The philosophy of the proposed modeling scheme is based in two parts: determining the equilibrium orientation of the wafer and calculation of wear and heat transfer in that orientation.

B.3.1 Equilibrium orientation

The balancing of all the external loads on the wafer results in the wafer achieving dynamic equilibrium. The major forces that act on the wafer are: hydrodynamic pressure, contact stress, friction and the external polishing load. Additional details

about balancing are available in a companion paper by Srivastava and Higgs [144] .

B.3.2 Wear calculation

The total wear calculation follows the algorithm proposed by Luo and Dornfeld [73]. The number of active particles is calculated based on the contact stress distribution and multiplied by the average wear (the wear caused by an average sized active particle), to determine the total wear at that instant.

B.3.3 Temperature calculation

The temperature evolution process can be broken down into three steps

1. Heat generation at the interface
2. Heat diffusion into the wafer and the pad
3. Heat extraction by the slurry

The primary mechanism for heat addition into the system has been assumed to be the frictional heat generation at the asperity contacts (viscous heat generation in the fluid is considered, but other sources such as plastic deformation have been neglected). This heat generated at the asperity tip is then distributed among the pad and the wafer asperities in contact. Following Blok's Conjecture [145], it is assumed that the flash temperature of the wafer asperity tip is the same as that of the pad asperity tip. Hence, the nominal temperatures of the two bodies, together with their material properties dictate the partition of heat among the two bodies, which is governed by equation (B.2). Further, it is assumed that the wafer-slurry-pad system has been insulated from the surroundings, and there is no external sink for dissipation of the

generated heat. This assumption allows us to simplify our system, at the same time helping us set up reasonable boundary conditions. The diffusion of frictional heat into the solids is governed by the transient heat conduction equation (B.3), which is independently solved for the pad and the wafer in their own coordinate systems.

A lubrication approximation of the three dimensional steady-state energy equation shown in eq (B.1) has been solved [146] to model the thermal transport through the slurry. The temperatures of the pad and the wafer act as the boundary conditions for the energy equation. In return, the fluid acts as a heat source or a sink for the two solid bodies. The fluid acts as a source or a sink depending on the temperature profile within the fluid.

The temperature distribution in the fluid is solved through the three dimensional energy equation, that is simplified by applying the thin fluid film assumption:

$$\begin{aligned}
 \rho C_v \left(\frac{\partial T}{\partial t} + u_r \frac{\partial T}{\partial r} + \frac{u_\theta}{r} \frac{\partial T}{\partial \theta} + u_z \frac{\partial T}{\partial z} \right) = & \\
 \frac{1}{r} \frac{\partial}{\partial r} \left(r k \frac{\partial T}{\partial r} \right) + \frac{1}{r^2} \frac{\partial}{\partial \theta} \left(k \frac{\partial T}{\partial \theta} \right) + \frac{\partial}{\partial z} \left(k \frac{\partial T}{\partial z} \right) - & \\
 T \frac{\partial P}{\partial T} \Big|_p \left(\frac{1}{r} \frac{\partial}{\partial r} (r u_r) + \frac{1}{r} \frac{\partial u_\theta}{\partial \theta} + \frac{\partial u_z}{\partial z} \right) - & \\
 \tau_{rr} \frac{\partial u_r}{\partial r} - \tau_{\theta\theta} \frac{1}{r} \left(\frac{\partial u_\theta}{\partial \theta} + u_r \right) - \tau_{zz} \frac{\partial u_z}{\partial z} - & \\
 \tau_{r\theta} \left(r \frac{\partial}{\partial r} \left(\frac{u_\theta}{r} \right) + \frac{1}{r} \frac{\partial u_r}{\partial \theta} \right) - \tau_{rz} \left(\frac{\partial u_z}{\partial r} + \frac{\partial u_r}{\partial z} \right) - \tau_{\theta z} \left(\frac{1}{r} \frac{\partial u_z}{\partial \theta} + \frac{\partial u_\theta}{\partial z} \right) + G_e &
 \end{aligned}
 \tag{B.1}$$

$$\dot{Q}_f = \dot{Q}_w + \dot{Q}_p \tag{B.2}$$

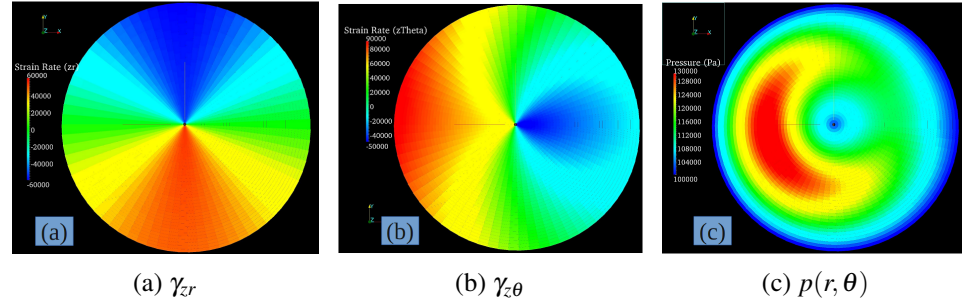


Figure B.1: Dependence of interfacial fluid pressure on shear-rate

$$\rho_i C_i \frac{\partial T}{\partial t} = k_i \nabla^2 T_i + \dot{q}_i \quad (\text{B.3})$$

B.4 Results

B.4.1 Hydrodynamic pressure

The quasi-steady state equilibrium orientation provides us the rolling angle, the pitching angle and the nominal clearance. These orientation parameters are then used to calculate the film thickness and after solving the Reynolds lubrication equation, the hydrodynamic pressure between the wafer and the pad. The hydrodynamic pressure strongly depends on the velocities of the two bounding surfaces. Figures B.1a and B.1b show the shear-rates (γ_{zr} , $\gamma_{z\theta}$ respectively) and the associated pressure field (Fig. B.1c) for certain values of the orientation parameters. From Fig. B.1c it seems that the pressure field can be obtained by adding the two shear rates together. Note that $\gamma_{z\theta}$ clearly dominates the resultant as it has higher overall variation. This scheme of hydrodynamic pressure calculation has been validated earlier by Srivastava and Higgs [7].

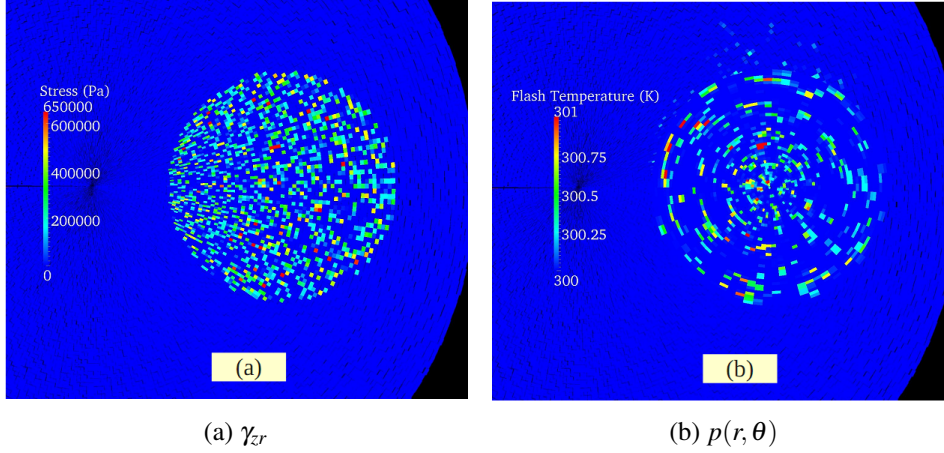


Figure B.2: (a) Variation in contact stress in the pad, (b) Corresponding flash temperatures

B.4.2 Contact stress

The wafer is assumed to be rigid and relatively smooth as compared to the pad. The orientation parameters also allow us to calculate the deformation, which due to its higher elasticity, exists only in the pad. This deformation then, through the constitutive relations, provides the contact stress distribution between the wafer and the pad. Higher contact stresses mean higher frictional heat generation, and thus, higher local temperatures. Fig. B.2a shows the contact stress field on the pad.

B.4.3 Temperature map

Figures B.3a and B.3b show the pad and wafer temperature distribution at an instant of simulation. As the thermal conductivity of the wafer is much higher than the pad, a larger fraction of the frictional heat gets transmitted on to the wafer. This difference can be clearly seen in the range of temperature values attained by the two bodies. Also, the thermal capacity of the wafer is much lower than that of the

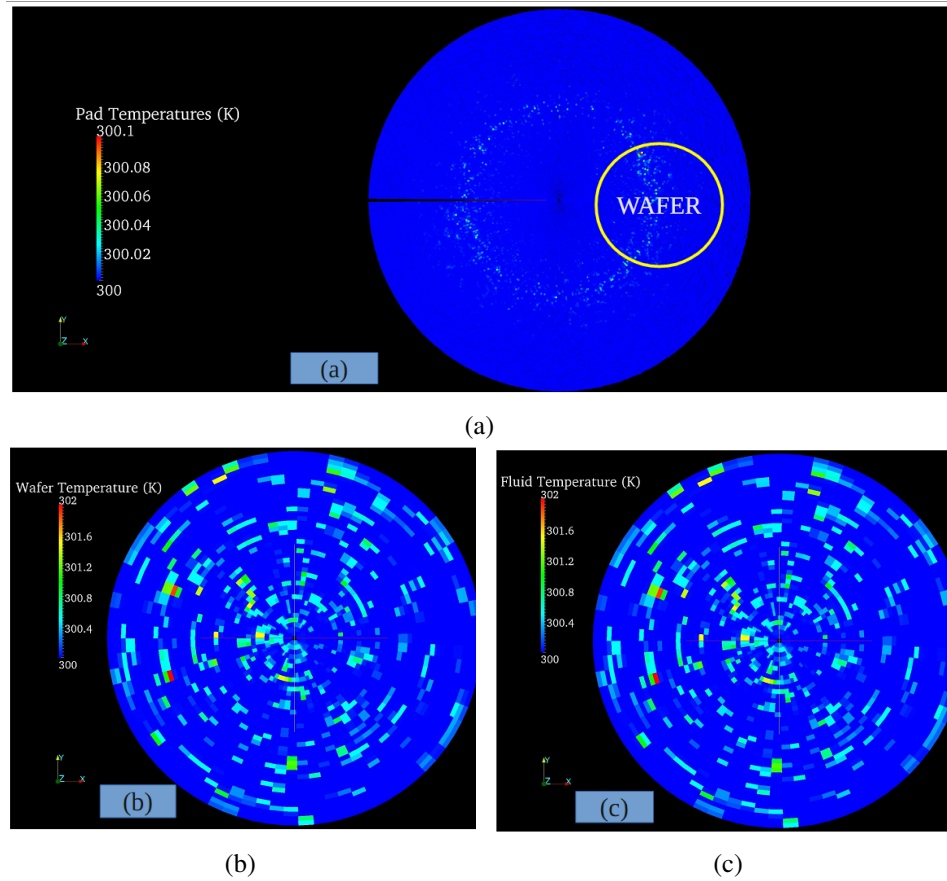


Figure B.3: Temperature maps (a) Pad temperatures (b) Wafer temperatures (c) Interfacial fluid film temperatures

pad, meaning that every element of the pad has a higher capacity to store the energy within itself, before diffusing the energy to its neighbors. As a result of this, the spatial variation across the wafer is also smoother than that of the pad. The reason that the temperature distributions are not as smooth as one might expect, is due to the fact that the results are shown for short simulation times and there is a significant disparity in thermal conductivities of the three materials (i.e., pad, wafer and slurry).

B.4.4 Parametric study: Slurry viscosity

The effect of changing the viscosity on the wafer average temperature and material removal rate was studied. Viscosity was chosen as a parameter, as it affects both the equilibrium orientation and the heat transfer. By changing the hydrodynamic pressure, viscosity affects the equilibrium orientation, and by changing the viscous heat generation in the fluid, it affects the temperatures.

As seen in Fig. B.4, increasing the viscosity increases the temperature. Expectedly, increase in the viscosity increases the viscous heat generation in the fluid, which leads to lesser heat extraction from the wafer. This is followed parallel with an increase in the material removal rate. It is likely that with increasing viscosity we are somehow seeing an increase in the contact stresses which would affect both the heat generation and material removal rate. However, notice that the temperature rises only up to a certain point (0.008 Pa-s). At that point, as the MRR drops, it is possible that the hydrodynamic pressure became high enough and a larger part of the applied load was being supported by the fluid. This resulted in lower contact stress, thus reducing the material removal and frictional heat generation, in turn reducing the average temperature.

B.5 Conclusion

A new framework for modeling thermal effects during CMP has been presented. The temperature is predicted by calculating the diffusion of frictional heat into the wafer and the pad, and extraction of the diffused heat by the slurry. The three-dimensional energy equation has been solved to study the thermal transport through

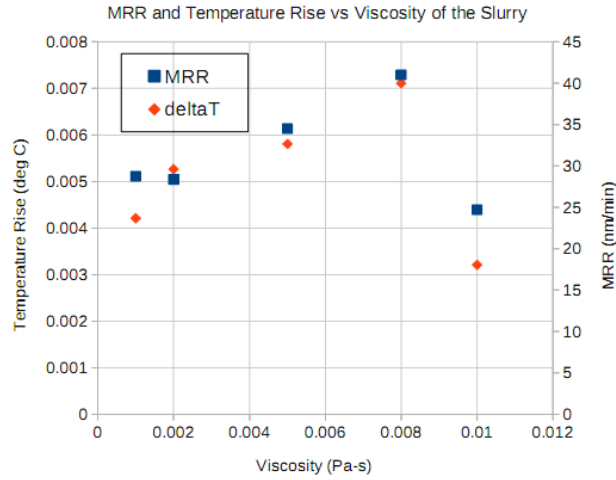


Figure B.4: Variation in temperature rise and MRR with viscosity

the fluid. The new framework can give us detailed information about the thermal behavior of the wafer-slurry-pad interface. It can also be used to study dependence of temperature change on different CMP parameters.

Appendix C

Titanium Polishing in the Antek Stretch Polisher

C.1 Introduction

Titanium is a relatively new metal and expensive to produce, but its outstanding properties of high strength to weight ratio and excellent corrosion and heat resistance have made titanium and its alloys well established engineering materials. Titanium is exceptionally resistant to corrosion by a wide range of chemicals. Its high affinity for oxygen results in a thin, but dense, self-healing stable oxide layer, which provides an effective barrier against incipient corrosion. In addition, it is the high strength to weight ratio maintained at elevated temperatures, which makes titanium and its alloys attractive for many critical applications. Titanium and its alloys are widely used in the aerospace and aircraft, chemical and medical industry, where high safety is essential. Consequently, specific study of Titanium processing is important.

C.2 Literature Review

A thorough literature review was conducted at the beginning of the project. The primary purpose was to gain insight in the current state of the art methods of Titanium processing, ultra-thin substrate handling and polishing and an overview of methods employed for achieving ultra-smooth surface finish.

It was discovered that ultra-thin substrates are being polished through CMP for a while. Majority of researchers have used mechanical handles, typically in the form of secondary, carrier wafers to facilitate handling of ultra-thin ($< 100\mu m$ thick) substrates. The two samples are bonded through a temporary bond or adhesive that can be easily removed after lapping and polishing.

Another important fact that appeared prominently across the board, was that to achieve very low roughness values ($< 10nm$) multi-stage polishing is essential. This is most commonly performed in two or three stages, with the earlier stages utilizing coarse grained, hard abrasives such as diamond or alpha-Alumina based slurries. This step results in lower roughness ($10 - 100nm$ depending on the conditions) than the initial surface and also results in a larger material removal rate. The final, finishing step usually employs softer, finer abrasives in the form of colloidal silica to achieve a much smoother surface ($\sim 1nm$). Aside from the size of the abrasives, the difference between the steps also lies in the mechanism of material removal. The earlier steps have larger influence of the 'chemical' aspect of the polishing, whereas the final polishing step is an almost purely mechanical process.

C.3 Sample Preparation

Titanium is a very ductile metal and prone to mechanical deformation. For the abrasive processes in metallographic cutting, grinding and polishing, this aspect has to be taken into consideration. While cutting, titanium can overheat and form large burrs and this also results in large deformations and scratches while grinding or polishing.

The material is obtained from the producer is obtained in the form of sheets. Because of the unusual properties discussed above, obtaining to-be-polished wafers out of these sheets is also a fairly difficult task. Initially conventional methods of cutting thin sheets, such as hole-saws were attempted. However, as mentioned earlier, due to its high ductility extremely large burrs were formed on the edges, rendering the cut wafers completely useless. Eventually, specific thin-sample machining processes were tried: wire EDM was tested by Antek and abrasive water-jet machining was tested by the PFTL. Among the two, as seen in a sample comparison picture below (fig ??, wire EDM produced a better edge finish. However, with its faster processing speed, lesser heating effects, lower contamination and overall lesser cost, water-jet cutting was deemed as a better option of the two.

C.4 Handling

Following the numerous studies found during the literature review that were processing thin wafers, "mechanical handles" based approach was used for holding the thin (thickness $\sim 50\mu m$) Titanium wafers. Several bonding agents and carrier wafers were tested. Earlier 4 inch wafers were cut out of the sheets but were later switched with 2.5 inch ones. The smaller wafers were more economical, easier to

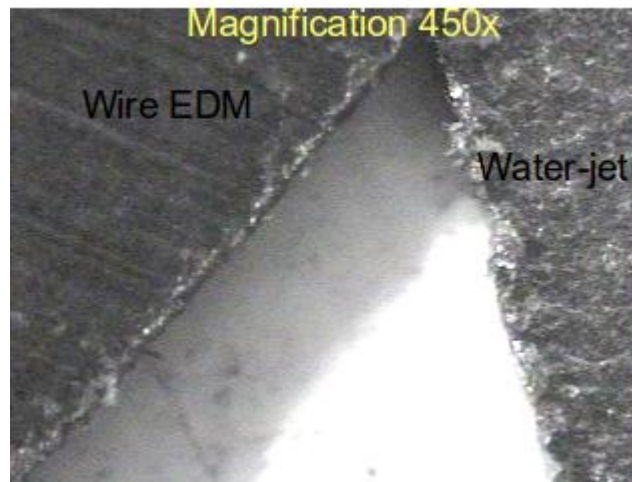


Figure C.1: Comparison in edge quality of wafers obtained through abrasive water-jet cutting and wire EDM

bond uniformly and matched the size of the wafers in the final application.

Different bonding methods tested ranged from the simpler double-sided tape and spray-bond adhesive to more complex hot-waxes. Eventually hot-melt-wax manufactured in 'sheet' form was found to yield the best polishing results. The near-uniform thickness of the sheet resulted in more uniform thickness of the bond, thus yielding more uniformly polished wafer. The wax was dissolved in Toluene after operation for debonding the samples.

A variety of carrier wafers were also tested for optimum operation. As was studied in the literature review, the first samples tried were metallic carriers, primarily mild steel and cast iron. Its low cost and good thermal properties made it an ideal candidate. However, it turned out extremely difficult to find very 'flat' samples. In most cases, the inherent curvature of the carriers led to the Titanium wafer getting delaminated from the carrier, leading to no polishing. To obtain 'flatness', Silicon wafers were tried next, which were also the next cheaper alternative. However, their

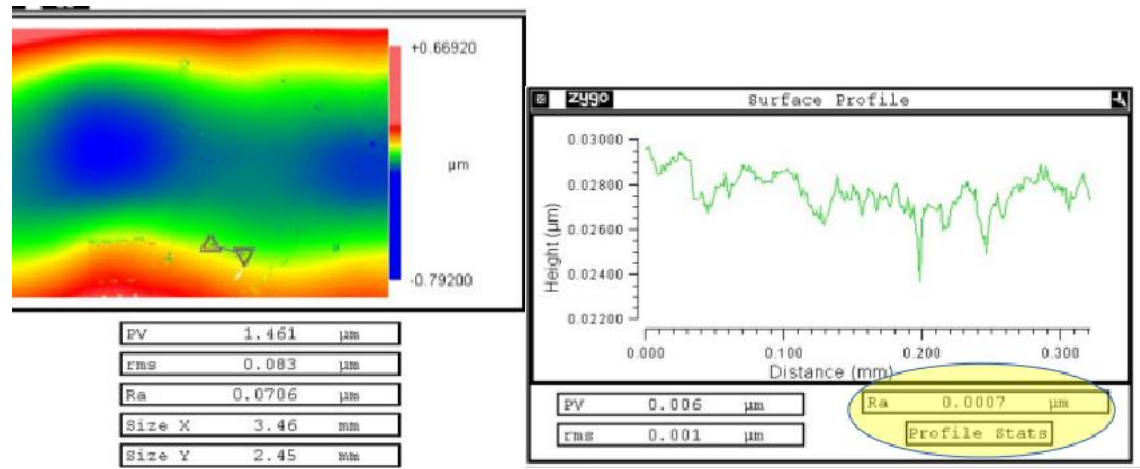
poor thermal properties made uniform bonding difficult, again resulting in delamination of the Titanium wafers. Mechanically, they were quite brittle and occasionally cracked during polishing. Finally glass wafers were found to be the best carriers. Although their price was slightly higher than plane Silicon wafers, their thermal and mechanical properties were more favorable than the other alternatives. As a bonus, because of their transparency, it was easier to spot and rectify bonding defects.

C.5 Recipe Recommendation

It was observed during the literature review that almost all researchers employ multi-step polishing to achieve ultra-smooth surfaces.

Similar to the literature, the first step consisted of larger tougher abrasives. The abrasives used for this study were alumina (Al_2O_3) and ceria (CeO_2). An oxidizing agent was added to expedite the dissolution of Ti as TiO_2 . Typically hydrogen peroxide (H_2O_2) or potassium permanganate (KMnO_4) is added. Higher pH, or hydroxide content (OH^-) also accelerates this reaction. For this purpose, KOH was added to the slurry. Polishing with the resulting slurry leads to a higher material removal rate, and a higher surface roughness.

The second polishing step is then used to reduce the high average roughness after the first step. Smaller, softer abrasives are used in the slurry. Typically silica based slurries are useful for this purpose. Usually no additives are added to the default slurry, which results in a purely mechanical polishing process, yielding a very low material removal rate and ultra-low surface roughness. Again, if higher material removal rate is required some oxidizing agent can be added.



(a) Profile over a section of the wafer

(b) Profile along a line

Figure C.2: Surface profile of a polished surface extracted from Zygo NuView 6300 optical profilometer

WARNING: The user is strongly advised to NOT attempt to alter the pH of any silica based slurry. Silicates coagulate and form large clumps in presence of protons (H^+ ions), which is what happens if you disturb the pH.

The figure C.2 shows a sample result of polishing with the Cabot Microelectronics slurry C7092, which is alumina based, with 6% hydrogen peroxide and a pH of 10.1. As the scan shows, there is a significant waviness in the surface, but local roughness is low (0.7 nm).

C.6 Modeling

Titanium polishing rates were first modeled using the PFTL's in-house benchtop polishing model called 'PAML+ for CMP'. The results of a typical temporal prediction are shown in figure C.3. The polishing parameters used for this study are listed

next to the material removal plot.

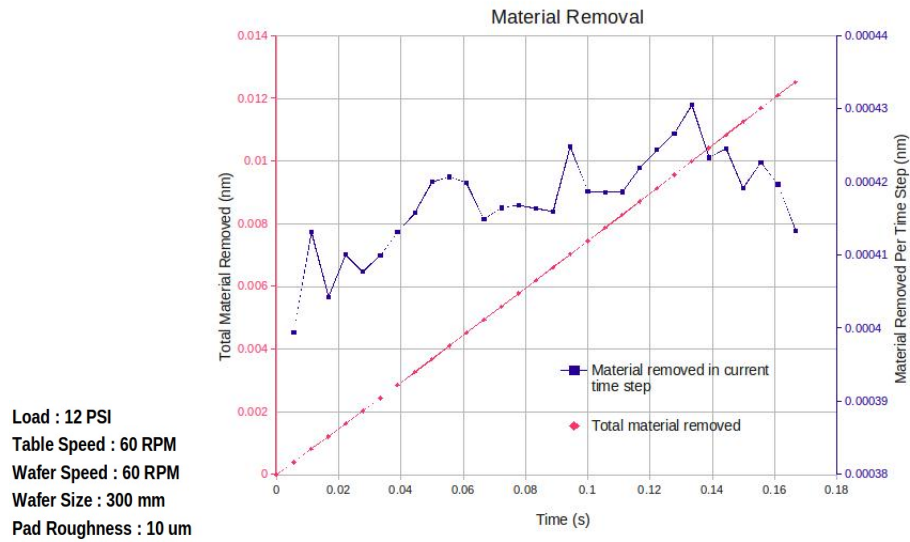


Figure C.3: Predictions of material removal using PAML+ for conventional polisher

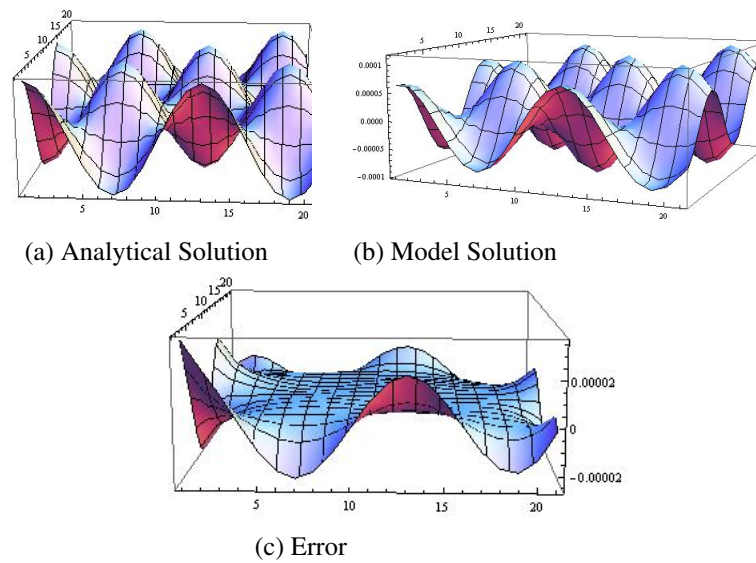


Figure C.4: Contact stress between a sinusoidal surface and another flat surface

PAML+ is a multi-physics model that combines the fluid, structural and wear

actions into one single framework. To improve the model predictions, the structural section of the model was modified for better calculation of the solid-solid contact stress acting between the wafer and the pad. Figure C.4 plots the contact stress for a sinusoidal surface contacting a flat surface, with (a) showing the analytical solution, (b) showing the new contact model. (c) shows the error between the model and the analytical solution.

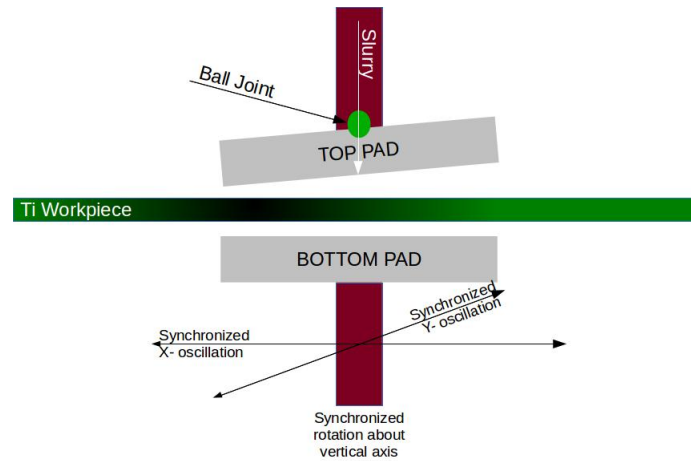


Figure C.5: Antek stretch polisher: major components and motions

The approach followed while constructing the PAML+ for CMP model was then applied to build a modeling framework for the Antek stretch polisher. Figure C.5 shows the major components and their operation in the machine. More details about the physical interactions captured by the model can be found in the appendix. Figure C.6 shows a screenshot of top-pad and the workpiece in the model.

Lastly, the material removal rates of only the "top-pad" in Antek stretch polisher were compared with the conventional polisher. Figure /reffig:Antekmrrspeed plots material removal rate as a function of rotation speed of the pad. It can be seen that with higher pad speed, stretch polisher increasingly performs better than the

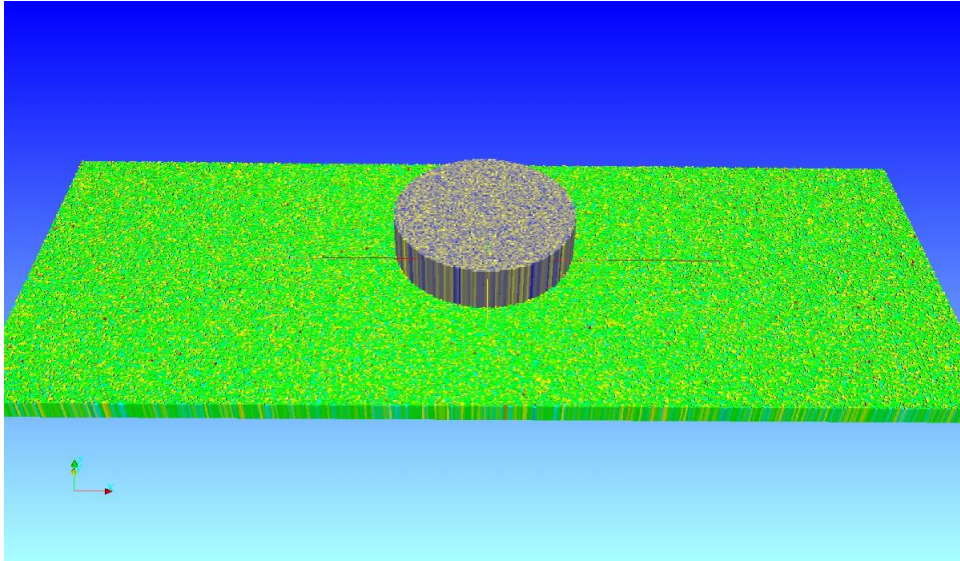


Figure C.6: PAML+ for Antek stretch polisher: sample output

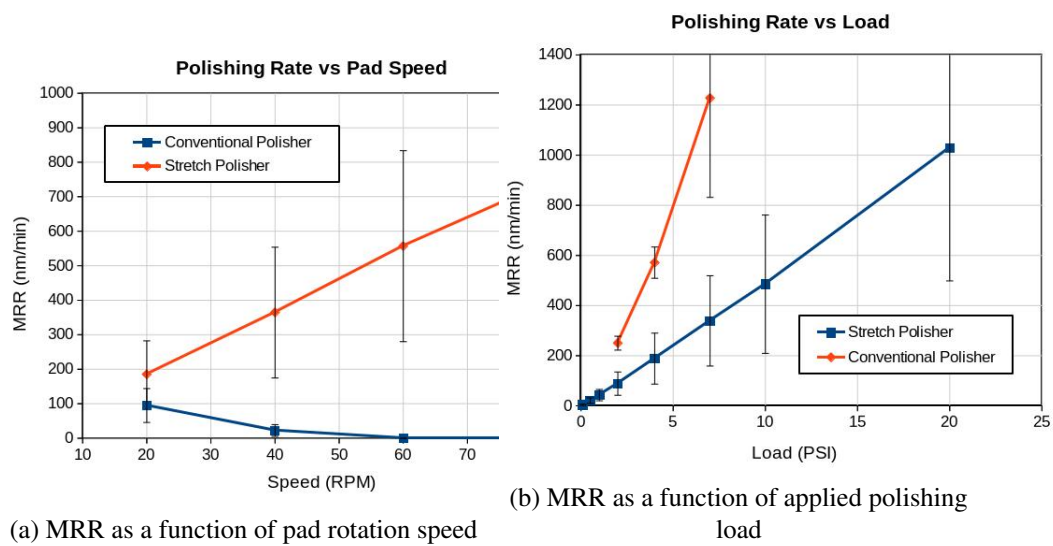


Figure C.7: Comparison of material removal rates between a conventional rotary polisher and the Antek stretch polisher

conventional polisher in terms of the material removal rate. Figure (b) plots the material removal rate as a function of the applied load, with the pad angular velocity fixed at 20 RPM. At higher loads, conventional polisher performs better than the stretch polisher. The under-performance of the stretch polisher can be attributed to the difference in area of the contact between the work-piece and the pad. In the case of conventional polisher, the entire workpiece is getting polished at the higher load, thus leading to higher material removal. Whereas, in the stretch polisher, a very small section of the workpiece (area of the polishing pad) is being polished by the higher load, with majority of the workpiece out of contact. As a result, the difference in average material removal in the case of the stretch-polisher is much lower than the conventional polisher, upon increasing the applied load.

Bibliography

- [1] H. A. Spikes, “Mixed lubrication — an overview,” *Lubrication Science*, vol. 9, pp. 221–253, May 1997.
- [2] W. Karunasena, C. M. Wang, S. Kitipornchai, and Y. Xiang, “Exact solutions for axisymmetric bending of continuous annular plates,” *Computers & Structures*, vol. 63, pp. 455–464, May 1997.
- [3] F. W. PRESTON, “The Theory and Design of Plate Glass Polishing Machines,” *J. Soc. Glass Tech.*, vol. 11, p. 214, 1927.
- [4] J. F. Archard, “Contact and Rubbing of Flat Surfaces,” *Journal of Applied Physics*, vol. 24, pp. 981–988, Aug. 1953.
- [5] A. Cameron, *The principles of lubrication: by A. Cameron*. London: Longmans, 1966.
- [6] J. A. Greenwood and J. B. P. Williamson, “Contact of Nominally Flat Surfaces,” *Proceedings of the Royal Society of London A: Mathematical, Physical and Engineering Sciences*, vol. 295, pp. 300–319, Dec. 1966.

- [7] N. Patir and H. S. Cheng, "Application of Average Flow Model to Lubrication Between Rough Sliding Surfaces," *Journal of Lubrication Technology*, vol. 101, pp. 220–229, Apr. 1979.
- [8] N. Patir and H. S. Cheng, "An Average Flow Model for Determining Effects of Three-Dimensional Roughness on Partial Hydrodynamic Lubrication," *Journal of Lubrication Technology*, vol. 100, pp. 12–17, Jan. 1978.
- [9] H. G. Elrod, "A General Theory for Laminar Lubrication With Reynolds Roughness," *Journal of Lubrication Technology*, vol. 101, pp. 8–14, Jan. 1979.
- [10] H. Christensen, "Some aspects of the functional influence of surface roughness in lubrication," *Wear*, vol. 17, pp. 149–162, Feb. 1971.
- [11] H. Christensen and K. Tonder, "The Hydrodynamic Lubrication of Rough Journal Bearings," *Journal of Lubrication Technology*, vol. 95, pp. 166–172, Apr. 1973.
- [12] T. E. Tallian, Y. P. Chiu, D. F. Huttenlocher, J. A. Kamenshine, L. B. Sibley, and N. E. Sindlinger, "Lubricant Films in Rolling Contact of Rough Surfaces," *A S L E Transactions*, vol. 7, pp. 109–126, Jan. 1964.
- [13] H. Czichos, "Untersuchungen über die verteilung metallischer und nichtmetallischer kontaktanteile bei mischreibung," *Wear*, vol. 17, pp. 209–217, Mar. 1971.
- [14] K. Johnson, J. Greenwood, and S. Poon, "A simple theory of asperity contact in elastohydro-dynamic lubrication," *Wear*, vol. 19, pp. 91–108, Jan. 1972.

- [15] T. E. Tallian, "The theory of partial elastohydrodynamic contacts," *Wear*, vol. 21, pp. 49–101, Aug. 1972.
- [16] J. A. Greenwood and J. H. Tripp, "The Contact of Two Nominally Flat Rough Surfaces," *Proceedings of the Institution of Mechanical Engineers*, vol. 185, pp. 625–633, June 1970.
- [17] L. Chang and M. N. Webster, "A Study of Elastohydrodynamic Lubrication of Rough Surfaces," *Journal of Tribology*, vol. 113, pp. 110–115, Jan. 1991.
- [18] K. Ichimaru and T. Morita, "Mechanism of direct contact and numerical model for analysis of line contact mixed elastohydrodynamic lubrication in pure rolling condition," *Journal of Japanese Society of Tribologists*, vol. 49, no. 1, pp. 83–91, 2004. WOS:000220270000015.
- [19] M. Scaraggi and B. N. J. Persson, "Time-Dependent Fluid Squeeze-Out Between Soft Elastic Solids with Randomly Rough Surfaces," *Tribology Letters*, vol. 47, pp. 409–416, Sept. 2012. WOS:000307295100009.
- [20] H. Qiao, H. P. Evans, and R. W. Snidle, "Comparison of fatigue model results for rough surface elastohydrodynamic lubrication," *Proceedings of the Institution of Mechanical Engineers Part J-Journal of Engineering Tribology*, vol. 222, pp. 381–393, May 2008. WOS:000256246700022.
- [21] A. A. Elsharkawy, M. J. A. Holmes, H. P. Evans, and R. W. Snidle, "Micro-elastohydrodynamic lubrication of coated cylinders using coupled differential deflection method," *Proceedings of the Institution of Mechanical Engineers Part J-Journal of Engineering Tribology*, vol. 220, pp. 29–41, Feb. 2006. WOS:000237790200003.

- [22] B. C. Majumdar and B. J. Hamrock, "Effect of Surface Roughness on Elastohydrodynamic Line Contact," *Journal of Lubrication Technology*, vol. 104, pp. 401–407, July 1982.
- [23] D. Zhu and H. S. Cheng, "Effect of Surface Roughness on the Point Contact EHL," *Journal of Tribology*, vol. 110, no. 1, p. 32, 1988.
- [24] D. Zhu, H. Cheng, T. Arai, and K. Hamai, "A Numerical-Analysis for Piston Skirts in Mixed Lubrication .1. Basic Modeling," *Journal of Tribology-Transactions of the Asme*, vol. 114, pp. 553–562, July 1992. WOS:A1992JF35300029.
- [25] L. Chang, M. Webster, and A. Jackson, "A Line-Contact Micro-Ehl Model with 3-Dimensional Surface-Topography," *Journal of Tribology-Transactions of the Asme*, vol. 116, pp. 21–28, Jan. 1994. WOS:A1994MU73400004.
- [26] G. Guangteng and H. Spikes, "An experimental study of film thickness in the mixed lubrication regime," *Tribology Series*, vol. 32, pp. 159–166, 1997.
- [27] M. Kaneta and H. Nishikawa, "Local Reduction in Thickness of Point Contact EHL Films Caused by a Transversely Oriented Moving Groove and Its Recovery," *Journal of Tribology*, vol. 116, pp. 635–639, July 1994.
- [28] M. HARTL, I. KŘUPKA, V. FUIS, and M. LIŠKA, "Experimental Study of Lubricant Film Thickness Behavior in the Vicinity of Real Asperities Passing through Lubricated Contact," *Tribology Transactions*, vol. 47, pp. 376–385, July 2004.

- [29] L. Chang, "A deterministic model for line-contact partial elastohydrodynamic lubrication," *Tribology International*, vol. 28, pp. 75–84, Mar. 1995.
- [30] X. Jiang, D. Y. Hua, H. S. Cheng, X. Ai, and S. C. Lee, "A Mixed Elastohydrodynamic Lubrication Model With Asperity Contact," *Journal of Tribology*, vol. 121, pp. 481–491, July 1999.
- [31] X. Jiang, H. S. Cheng, and D. Y. Hua, "A theoretical analysis of mixed lubrication by macro micro approach: Part I - Results in a gear surface contact," *Tribology Transactions*, vol. 43, pp. 689–699, Oct. 2000. WOS:000089475300019.
- [32] J. X. Zhao and F. Sadeghi, "The effects of a stationary surface pocket on EHL line contact start-up," *Journal of Tribology-Transactions of the Asme*, vol. 126, pp. 672–680, Oct. 2004. WOS:000225667500005.
- [33] J. X. Zhao, F. Sadeghi, and M. H. Hoeprich, "Analysis of EHL circular contact start up: Part I - Mixed contact model with pressure and film thickness results," *Journal of Tribology-Transactions of the Asme*, vol. 123, pp. 67–74, Jan. 2001. WOS:000166600100010.
- [34] M. J. A. Holmes, H. P. Evans, and R. W. Snidle, "Analysis of mixed lubrication effects in simulated gear tooth contacts," *Journal of Tribology-Transactions of the Asme*, vol. 127, pp. 61–69, Jan. 2005. WOS:000227266900008.
- [35] J. X. Zhao and F. Sadeghi, "Analysis of EHL circular contact shut down," *Journal of Tribology-Transactions of the Asme*, vol. 125, pp. 76–90, Jan. 2003. WOS:000180443200010.

- [36] G. Popovici, C. H. Venner, and P. M. Lugt, "Effects of load system dynamics on the film thickness in EHL contacts during start up," *Journal of Tribology-Transactions of the Asme*, vol. 126, pp. 258–266, Apr. 2004. WOS:000220934900006.
- [37] Y.-Z. Hu and D. Zhu, "A Full Numerical Solution to the Mixed Lubrication in Point Contacts," *Journal of Tribology*, vol. 122, pp. 1–9, June 1999.
- [38] M. J. A. Holmes, H. P. Evans, T. G. Hughes, and R. W. Snidle, "Transient elastohydrodynamic point contact analysis using a new coupled differential deflection method. Part 1: theory and validation," *Proceedings of the Institution of Mechanical Engineers Part J-Journal of Engineering Tribology*, vol. 217, no. J4, pp. 289–303, 2003. WOS:000185543300004.
- [39] M. J. A. Holmes, H. P. Evans, T. G. Hughes, and R. W. Snidle, "Transient elastohydrodynamic point contact analysis using a new coupled differential deflection method. Part 2: results," *Proceedings of the Institution of Mechanical Engineers Part J-Journal of Engineering Tribology*, vol. 217, no. J4, pp. 305–321, 2003. WOS:000185543300005.
- [40] S. Li and A. Kahraman, "A mixed EHL model with asymmetric integrated control volume discretization," *Tribology International*, vol. 42, pp. 1163–1172, Aug. 2009. WOS:000267731700005.
- [41] S. Li and A. Kahraman, "A Transient Mixed Elastohydrodynamic Lubrication Model for Spur Gear Pairs," *Journal of Tribology-Transactions of the Asme*, vol. 132, p. 011501, Jan. 2010. WOS:000272613400007.

- [42] A. A. Polycarpou and A. Soom, "A two-component mixed friction model for a lubricated line contact," *Journal of Tribology-Transactions of the Asme*, vol. 118, pp. 183–189, Jan. 1996. WOS:A1996UF83400024.
- [43] E. R. M. Gelinck and D. J. Schipper, "Calculation of Stribeck curves for line contacts," *Tribology International*, vol. 33, pp. 175–181, Apr. 2000.
- [44] N. Ren, D. Zhu, W. W. Chen, Y. Liu, and Q. J. Wang, "A Three-Dimensional Deterministic Model for Rough Surface Line-Contact EHL Problems," *Journal of Tribology*, vol. 131, pp. 011501–011501, Dec. 2008.
- [45] S. L. W. Wayne Chen, "Fast Fourier Transform Based Numerical Methods for ElastoPlastic Contacts of Nominally Flat Surfaces," *Journal of Applied Mechanics-transactions of The Asme - J APPL MECH*, vol. 75, no. 1, 2008.
- [46] W.-Z. Wang, Y.-C. Liu, H. Wang, and Y.-Z. Hu, "A Computer Thermal Model of Mixed Lubrication in Point Contacts," *Journal of Tribology*, vol. 126, pp. 162–170, Jan. 2004.
- [47] H. Sojoudi and M. M. Khonsari, "On the Behavior of Friction in Lubricated Point Contact With Provision for Surface Roughness," *Journal of Tribology*, vol. 132, pp. 012102–012102, Nov. 2009.
- [48] Z. M. Jin, "Analysis of mixed lubrication mechanism in metal-on-metal hip joint replacements," *Proceedings of the Institution of Mechanical Engineers, Part H: Journal of Engineering in Medicine*, vol. 216, pp. 85–89, Jan. 2002.
- [49] S. L. Smith, D. Dowson, A. a. J. Goldsmith, R. Valizadeh, and J. S. Colligon, "Direct evidence of lubrication in ceramic-on-ceramic total hip replacements,"

Proceedings of the Institution of Mechanical Engineers, Part C: Journal of Mechanical Engineering Science, vol. 215, pp. 265–268, Mar. 2001.

- [50] A. Wang, A. Essner, V. K. Polineni, C. Stark, and J. H. Dumbleton, “Lubrication and wear of ultra-high molecular weight polyethylene in total joint replacements,” *Tribology International*, vol. 31, pp. 17–33, Jan. 1998.
- [51] F. C. Wang and Z. M. Jin, “Prediction of elastic deformation of acetabular cups and femoral heads for lubrication analysis of artificial hip joints,” *Proceedings of the Institution of Mechanical Engineers, Part J: Journal of Engineering Tribology*, vol. 218, pp. 201–209, Mar. 2004.
- [52] W.-Z. Wang, F.-C. Wang, Z.-M. Jin, D. Dowson, and Y.-Z. Hu, “Numerical lubrication simulation of metal-on-metal artificial hip joint replacements: ball-in-socket model and ball-on-plane model,” *Proceedings of the Institution of Mechanical Engineers Part J-Journal of Engineering Tribology*, vol. 223, pp. 1073–1082, Nov. 2009. WOS:000272988700018.
- [53] F. C. Wang, C. Brockett, S. Williams, I. Udofia, J. Fisher, and Z. M. Jin, “Lubrication and friction prediction in metal-on-metal hip implants,” *Physics in Medicine and Biology*, vol. 53, p. 1277, Mar. 2008.
- [54] O. Akalin and G. M. Newaz, “Piston ring-cylinder bore friction modeling in mixed lubrication regime: Part I - Analytical results,” *Journal of Tribology-Transactions of the Asme*, vol. 123, pp. 211–218, Jan. 2001. WOS:000166600100028.

- [55] G. A. Livanos and N. P. Kyrtatos, "Friction model of a marine diesel engine piston assembly," *Tribology International*, vol. 40, pp. 1441–1453, Dec. 2007. WOS:000249878100005.
- [56] C. Priestner, H. Allmaier, H. H. Priebsch, and C. Forstner, "Refined simulation of friction power loss in crank shaft slider bearings considering wear in the mixed lubrication regime," *Tribology International*, vol. 46, pp. 200–207, Feb. 2012. WOS:000298534100023.
- [57] Z. Ma, N. A. Henein, and W. Bryzik, "A model for wear and friction in cylinder liners and piston rings," *Tribology Transactions*, vol. 49, pp. 315–327, Sept. 2006. WOS:000239950500004.
- [58] L. Shan, J. Levert, L. Meade, J. Tichy, and S. Danyluk, "Interfacial Fluid Mechanics and Pressure Prediction in Chemical Mechanical Polishing," *Journal of Tribology*, vol. 122, pp. 539–543, July 1999.
- [59] J. Seok, C. P. Sukam, A. T. Kim, J. A. Tichy, and T. S. Cale, "Multiscale material removal modeling of chemical mechanical polishing," *Wear*, vol. 254, pp. 307–320, Feb. 2003.
- [60] X. Q. Jin, L. M. Keer, and Q. Wang, "A 3d EHL simulation of CMP - Theoretical framework of modeling," *Journal of the Electrochemical Society*, vol. 152, no. 1, pp. G7–G15, 2005. WOS:000225864900064.
- [61] E. J. Terrell and C. F. Higgs III, "A Particle-Augmented Mixed Lubrication Modeling Approach to Predicting Chemical Mechanical Polishing," *Journal of Tribology*, vol. 131, no. 1, p. 012201, 2009.

- [62] G. Srivastava and C. F. Higgs, "A Full Wafer-Scale PAML Modeling Approach for Predicting CMP," *Tribology Letters*, vol. 59, pp. 1–11, June 2015.
- [63] W. Hodge, R. Fijan, K. Carlson, R. Burgess, W. Harris, and R. Mann, "Contact Pressures in the Human Hip-Joint Measured In vivo," *Proceedings of the National Academy of Sciences of the United States of America*, vol. 83, pp. 2879–2883, May 1986. WOS:A1986C174100022.
- [64] I. D. Learmonth, C. Young, and C. Rorabeck, "The operation of the century: total hip replacement," *Lancet (London, England)*, vol. 370, pp. 1508–1519, Oct. 2007.
- [65] G. Dearnaley and J. H. Arps, "Biomedical applications of diamond-like carbon (DLC) coatings: A review," *Surface and Coatings Technology*, vol. 200, pp. 2518–2524, Dec. 2005.
- [66] K. Beschorner, C. F. Higgs III, and M. Lovell, "Solution of Reynolds Equation in Polar Coordinates Applicable to Nonsymmetric Entrainment Velocities," *Journal of Tribology*, vol. 131, no. 3, p. 034501, 2009.
- [67] K. L. . Johnson, "Contact mechanics," 1985.
- [68] P. B. Zantye, A. Kumar, and A. Sikder, "Chemical mechanical planarization for microelectronics applications," *Materials Science and Engineering: R: Reports*, vol. 45, pp. 89–220, Oct. 2004.
- [69] Z. Zhang, W. Liu, Z. Song, and X. Hu, "Two-Step Chemical Mechanical Polishing of Sapphire Substrate," *Journal of The Electrochemical Society*, vol. 157, no. 6, p. H688, 2010.

- [70] H. Zhu, L. A. Tassaroto, R. Sabia, V. A. Greenhut, M. Smith, and D. E. Niesz, "Chemical mechanical polishing (CMP) anisotropy in sapphire," *Applied Surface Science*, vol. 236, pp. 120–130, Sept. 2004.
- [71] H. Lei and J. Luo, "CMP of hard disk substrate using a colloidal SiO₂ slurry: preliminary experimental investigation," *Wear*, vol. 257, pp. 461–470, Sept. 2004.
- [72] Y. Zhao and L. Chang, "A micro-contact and wear model for chemical–mechanical polishing of silicon wafers," *Wear*, vol. 252, no. 3, pp. 220–226, 2002.
- [73] J. Luo and D. A. Dornfeld, "Material removal mechanism in chemical mechanical polishing: theory and modeling," *Semiconductor Manufacturing, IEEE Transactions on*, vol. 14, no. 2, pp. 112–133, 2001.
- [74] J. N. Mpagazehe and C. F. Higgs, "A Comparison of Active Particle Models for Chemical Mechanical Polishing," *ECS Journal of Solid State Science and Technology*, vol. 2, pp. P87–P96, Jan. 2013.
- [75] S. Sundararajan, D. G. Thakurta, D. W. Schwendeman, S. P. Murarka, and W. N. Gill, "Two-dimensional wafer-scale chemical mechanical planarization models based on lubrication theory and mass transport," *Journal of the Electrochemical Society*, vol. 146, pp. 761–766, Feb. 1999. WOS:000078866400057.
- [76] S. Runnels, "Feature-Scale Fluid-Based Erosion Modeling for Chemical-Mechanical Polishing," *Journal of the Electrochemical Society*, vol. 141, pp. 1900–1904, July 1994. WOS:A1994NX19600040.

- [77] S. S. Park, C. H. Cho, and Y. Ahn, "Hydrodynamic analysis of chemical mechanical polishing process," *Tribology International*, vol. 33, pp. 723–730, Oct. 2000. WOS:000165311500005.
- [78] C. H. Cho, S. S. Park, and Y. Ahn, "Three-dimensional wafer scale hydrodynamic modeling for chemical mechanical polishing," *Thin Solid Films*, vol. 389, pp. 254–260, June 2001. WOS:000169378200038.
- [79] J. F. Luo and D. A. Dornfeld, "Effects of abrasive size distribution in chemical mechanical planarization: Modeling and verification," *Ieee Transactions on Semiconductor Manufacturing*, vol. 16, pp. 469–476, Aug. 2003. WOS:000184695600019.
- [80] A. Osorno, *Dynamic, In-Situ Pressure Measurements during CMP*. Thesis, Georgia Institute of Technology, Sept. 2005. M.S.
- [81] M. Biemann, "Effect of Particle Size during Tungsten Chemical Mechanical Polishing," *Electrochemical and Solid-State Letters*, vol. 2, no. 8, p. 401, 1999.
- [82] J. Luo and D. Dornfeld, "Material removal regions in chemical mechanical planarization for submicron integrated circuit fabrication: coupling effects of slurry chemicals, abrasive size distribution, and wafer-pad contact area," *IEEE Transactions on Semiconductor Manufacturing*, vol. 16, pp. 45–56, Feb. 2003.
- [83] E. Y. A. Worniyoh, V. K. Jasti, and I. Fred Higgs, C., "A Review of Dry Particulate Lubrication: Powder and Granular Materials," *Journal of Tribology*, vol. 129, pp. 438–449, Jan. 2007.

- [84] C. F. Higgs and J. Tichy, "Effect of particle and surface properties on granular lubrication flow," *Proceedings of the Institution of Mechanical Engineers, Part J: Journal of Engineering Tribology*, vol. 222, pp. 703–713, June 2008.
- [85] D. White, J. Melvin, and D. Boning, "Characterization and modeling of dynamic thermal behavior in CMP," *Journal of the Electrochemical Society*, vol. 150, pp. G271–G278, Apr. 2003. WOS:000181515100063.
- [86] L. Borucki, Z. Li, and A. Philipossian, "Experimental and theoretical investigation of heating and convection in copper polishing," *Journal of the Electrochemical Society*, vol. 151, no. 9, pp. G559–G563, 2004. WOS:000223622000065.
- [87] Z. Li, L. Borucki, I. Koshiyama, and A. Philipossian, "Effect of slurry flow rate on tribological, thermal, and removal rate attributes of copper CMP," *Journal of the Electrochemical Society*, vol. 151, no. 7, pp. G482–G487, 2004. WOS:000222676300067.
- [88] E. E. Remsen, S. Anjur, D. Boldridge, M. Kamiti, S. T. Li, T. Johns, C. Dowell, J. Kasthurirangan, and P. Feeney, "Analysis of large particle count in fumed silica slurries and its correlation with scratch defects generated by CMP," *Journal of the Electrochemical Society*, vol. 153, no. 5, pp. G453–G461, 2006. WOS:000236516000071.
- [89] G. K. McKee and J. Watson-Farrar, "Replacement of arthritic hips by the McKee-Farrar prosthesis.," *The Journal of bone and joint surgery. British volume*, vol. 48, pp. 245–59, May 1966. MEDLINE:5937593.

- [90] J. Charnley and Z. Cupic, "9 and 10 Year Results of Low-Friction Arthroplasty of Hip," *Clinical Orthopaedics and Related Research*, no. 95, pp. 9–25, 1973. WOS:A1973R500500002.
- [91] H. McKellop, P. Campbell, S. Park, T. Schmalzried, P. Grigoris, H. Amstutz, and A. Sarmiento, "The Origin of Submicron Polyethylene Wear Debris in Total Hip-Arthroplasty," *Clinical Orthopaedics and Related Research*, pp. 3–20, Feb. 1995. WOS:A1995QF55400002.
- [92] T. Schmalzried, L. Kwong, M. Jasty, R. Sedlacek, T. Haire, D. Oconnor, C. Bragdon, J. Kabo, A. Malcolm, M. Path, and W. Harris, "The Mechanism of Loosening of Cemented Acetabular Components in Total Hip-Arthroplasty - Analysis of Specimens Retrieved at Autopsy," *Clinical Orthopaedics and Related Research*, pp. 60–78, Jan. 1992. WOS:A1992GY54900009.
- [93] J. D. Mabrey, A. Afsar-Keshmiri, G. A. Engh, C. J. Sychterz, M. A. Wirth, C. A. Rockwood, and C. M. Agrawal, "Standardized analysis of UHMWPE wear particles from failed total joint arthroplasties," *Journal of Biomedical Materials Research*, vol. 63, no. 5, pp. 475–483, 2002.
- [94] P. Chen, E. Mead, J. Pinto, and C. Colwell, "Polyethylene Wear Debris in Modular Acetabular Prostheses," *Clinical Orthopaedics and Related Research*, pp. 44–56, Aug. 1995. WOS:A1995RP27300008.
- [95] T. Schmalzried, M. Jasty, and W. Harris, "Periprosthetic Bone Loss in Total Hip-Arthroplasty - Polyethylene Wear Debris and the Concept of the Effective Joint Space," *Journal of Bone and Joint Surgery-American Volume*, vol. 74A, pp. 849–863, July 1992. WOS:A1992JH48500006.

- [96] K. Hirakawa, T. W. Bauer, B. N. Stulberg, and A. H. Wilde, "Comparison and quantitation of wear debris of failed total hip and total knee arthroplasty," *Journal of Biomedical Materials Research*, vol. 31, pp. 257–263, June 1996. WOS:A1996UG00300013.
- [97] A. Kobayashi, W. Bonfield, Y. Kadoya, T. Yamac, M. a. R. Freeman, G. Scott, and P. A. Revell, "The size and shape of particulate polyethylene wear debris in total joint replacements," *Proceedings of the Institution of Mechanical Engineers Part H-Journal of Engineering in Medicine*, vol. 211, no. 1, pp. 11–15, 1997. WOS:A1997XB99300003.
- [98] D. W. Hahn, D. L. Wolfarth, and N. L. Parks, "Characterization of submicron polyethylene wear debris from synovial-fluid samples of revised knee replacements using a light-scattering technique," *Journal of Biomedical Materials Research*, vol. 31, pp. 355–363, July 1996. WOS:A1996UU78600009.
- [99] M. A. Wirth, C. M. Agrawal, J. D. Mabrey, D. D. Dean, C. R. Blanchard, M. A. Miller, and C. A. Rockwood, "Isolation and characterization of polyethylene wear debris associated with osteolysis following total shoulder arthroplasty," *Journal of Bone and Joint Surgery-American Volume*, vol. 81A, pp. 29–37, Jan. 1999. WOS:000078285600005.
- [100] R. M. Urban, J. J. Jacobs, M. J. Tomlinson, J. Gavrilovic, J. Black, and M. Peoc'h, "Dissemination of wear particles to the liver, spleen, and abdominal lymph nodes of patients with hip or knee replacement," *Journal of Bone and Joint Surgery-American Volume*, vol. 82A, pp. 457–477, Apr. 2000. WOS:000086193700002.

- [101] S. B. Goodman, J. A. Davidson, Y. Song, N. Martial, and V. L. Fornasier, "Histomorphological reaction of bone to different concentrations of phagocytosable particles of high-density polyethylene and Ti-6al-4v alloy in vivo," *Biomaterials*, vol. 17, pp. 1943–1947, Oct. 1996. WOS:A1996VJ53500003.
- [102] S. Goodman, V. Fornasier, J. Lee, and J. Kei, "The Histological Effects of the Implantation of Different Sizes of Polyethylene Particles in the Rabbit Tibia," *Journal of Biomedical Materials Research*, vol. 24, pp. 517–524, Apr. 1990. WOS:A1990CV88400007.
- [103] R. M. Hall, M. J. K. Bankes, and G. Blunn, "Biotribology for joint replacement," *Current Orthopaedics*, vol. 15, pp. 281–290, Aug. 2001. WOS:000174108600006.
- [104] D. Dowson, "Modes of lubrication in human joints," *ARCHIVE: Proceedings of the Institution of Mechanical Engineers, Conference Proceedings 1964-1970 (vols 178-184), Various titles labelled Volumes A to S*, vol. 181, pp. 45–54, June 1966.
- [105] X. Zhou, A. L. Galvin, Z. Jin, X. Yan, and J. Fisher, "The influence of concave dimples on the metallic counterface on the wear of ultra-high molecular weight polyethylene," *Proceedings of the Institution of Mechanical Engineers, Part J: Journal of Engineering Tribology*, vol. 226, pp. 455–462, Nov. 2011.
- [106] H. Ito, K. Kaneda, T. Yuhta, I. Nishimura, K. Yasuda, and T. Matsuno, "Reduction of polyethylene wear by concave dimples on the frictional surface

- in artificial hip joints,” *The Journal of Arthroplasty*, vol. 15, no. 3, pp. 332–338, 2000.
- [107] I. Etsion, “Improving tribological performance of mechanical components by laser surface texturing,” *Tribology Letters*, vol. 17, no. 4, p. 733–737, 2004.
- [108] A. Kovalchenko, O. Ajayi, A. Erdemir, G. Fenske, and I. Etsion, “The effect of laser texturing of steel surfaces and speed-load parameters on the transition of lubrication regime from boundary to hydrodynamic,” *Tribology Transactions*, vol. 47, pp. 299–307, Apr. 2004.
- [109] U. Pettersson and S. Jacobson, “Friction and wear properties of micro textured DLC coated surfaces in boundary lubricated sliding,” *Tribology letters*, vol. 17, no. 3, p. 553–559, 2004.
- [110] A. Ramesh, W. Akram, S. P. Mishra, A. H. Cannon, A. A. Polycarpou, and W. P. King, “Friction characteristics of microtextured surfaces under mixed and hydrodynamic lubrication,” *Tribology International*, vol. 57, pp. 170–176, Jan. 2013.
- [111] M. Jagatia and Z. M. Jin, “Elastohydrodynamic lubrication analysis of metal-on-metal hip prostheses under steady state entraining motion,” *Proceedings of the Institution of Mechanical Engineers, Part H: Journal of Engineering in Medicine*, vol. 215, pp. 531–541, June 2001.
- [112] F. Liu, Z. Jin, P. Roberts, and P. Grigoris, “Effect of bearing geometry and structure support on transient elastohydrodynamic lubrication of metal-on-metal hip implants,” *Journal of Biomechanics*, vol. 40, pp. 1340–1349, Jan. 2007.

- [113] L. M. Gao, Q. E. Meng, F. Liu, J. Fisher, and Z. M. Jin, "The effect of aspherical geometry and surface texturing on the elastohydrodynamic lubrication of metal-on-metal hip prostheses under physiological loading and motions," *Proceedings of the Institution of Mechanical Engineers, Part C: Journal of Mechanical Engineering Science*, vol. 224, pp. 2627–2636, Dec. 2010.
- [114] Z. M. Jin, "Theoretical studies of elastohydrodynamic lubrication of artificial hip joints," *Proceedings of the Institution of Mechanical Engineers, Part J: Journal of Engineering Tribology*, vol. 220, pp. 719–727, Jan. 2006.
- [115] T. P. Schmalzried, P. Campbell, A. K. Schmitt, I. C. Brown, and H. C. Amstutz, "Shapes and dimensional characteristics of polyethylene wear particles generated in vivo by total knee replacements compared to total hip replacements," *Journal of Biomedical Materials Research*, vol. 38, no. 3, pp. 203–210, 1997. WOS:A1997XT74200004.
- [116] A. G. Yew, D. Pinero, A. H. Hsieh, and J. Atencia, "Low Peclet number mass and momentum transport in microcavities," *Applied Physics Letters*, vol. 102, no. 8, p. 084108, 2013.
- [117] J. Livermore, D. Ilstrup, and B. Morrey, "Effect of femoral head size on wear of the polyethylene acetabular component," *The Journal of Bone and Joint Surgery. American Volume*, vol. 72, pp. 518–528, Apr. 1990.
- [118] T. A. Maxian, T. D. Brown, D. R. Pedersen, and J. J. Callaghan, "The Frank Stinchfield Award. 3-Dimensional sliding/contact computational simulation of total hip wear," *Clinical Orthopaedics and Related Research*, pp. 41–50, Dec. 1996.

- [119] T. A. Maxian, T. D. Brown, D. R. Pedersen, and J. J. Callaghan, "A sliding-distance-coupled finite element formulation for polyethylene wear in total hip arthroplasty," *Journal of Biomechanics*, vol. 29, pp. 687–692, May 1996.
- [120] J. S.-S. Wu, J.-P. Hung, C.-S. Shu, and J.-H. Chen, "The computer simulation of wear behavior appearing in total hip prosthesis," *Computer Methods and Programs in Biomedicine*, vol. 70, no. 1, pp. 81–91, 2003.
- [121] B. Ruan, R. F. Salant, and I. Green, "A mixed lubrication model of liquid/gas mechanical face seals," *Tribol. Trans.*, vol. 40, pp. 647–657, Oct. 1997. WOS:A1997YE97100015.
- [122] N. Brunetiere and B. Tournierie, "The effect of inertia on radial flows - Application to hydrostatic seals," *J. Tribol.-Trans. ASME*, vol. 128, pp. 566–574, July 2006. WOS:000239890300014.
- [123] N. Brunetiere, B. Tournierie, and J. Frene, "A simple and easy-to-use TEHD model for non-contacting liquid face seals," *Tribology Transactions*, vol. 46, no. 2, pp. 187–192, 2003.
- [124] B. Tournierie, N. Brunetiere, and J.-C. Danos, "2d numerical modelling of the TEHD transient behaviour of mechanical face seals," *Sealing Technology*, vol. 2003, pp. 10–13, June 2003.
- [125] N. Brunetire, "An analytical approach of the thermoelastohydrodynamic behaviour of mechanical face seals operating in mixed lubrication," *Proc. Inst. Mech. Eng. Part J J. Eng. Tribol.*, vol. 224, no. 12, pp. 1221–1233, 2010.

- [126] N. Brunetire and A. Apostolescu, "A simple approach to the thermoElasto-HydroDynamic behavior of mechanical face seals," *Tribol. Trans.*, vol. 52, no. 2, pp. 243–255, 2009.
- [127] C.-J. Liao, W.-F. Huang, Y.-M. Wang, S.-F. Suo, and X.-F. Liu, "Optimization design for mechanical seals in reactor coolant pumps based on a fluid-solid strong-interaction model," *Proceedings of the Institution of Mechanical Engineers, Part C: Journal of Mechanical Engineering Science*, vol. 225, pp. 1851–1862, June 2011.
- [128] C. Liao, W. Huang, S. Suo, X. Liu, and Y. Wang, "Fluid-solid strong-interaction model of mechanical seals in reactor coolant pumps," *Science China Technological Sciences*, vol. 54, pp. 2339–2348, Sept. 2011.
- [129] L. Xin, P. Xu-dong, and M. Xiang-kai, "Thermo-Elasto-Hydrostatic Effect Analysis of the Double Tapered Hydrostatic Mechanical Seals for Reactor Coolant Pumps under the Influence of Flow Regime," in *Power and Energy Engineering Conference (APPEEC), 2012 Asia-Pacific*, pp. 1–6, 2012.
- [130] N. Brunetiere, B. Tournierie, and J. Frene, "TEHD lubrication of mechanical face seals in stable tracking mode: Part 2-Parametric study," *Transactions of the ASME. Journal of Tribology*, vol. 125, pp. 617–27, July 2003.
- [131] E. Galenne and I. Pierre-Danos, "Thermo-elasto-hydro-dynamic Modeling of hydrostatic seals in reactor coolant pumps," *Tribol. Trans.*, vol. 50, pp. 466–476, Dec. 2007. WOS:000250684700004.

- [132] N. Brunetiere, B. Tournier, and J. Frene, "TEHD lubrication of mechanical face seals in stable tracking mode: Part 1 - Numerical model and experiments," *Journal of Tribology*, vol. 125, no. 3, pp. 608–616, 2003.
- [133] J. Danos, B. Tournier, and J. Frne, "THD lubrication of mechanical face seals during transient period after start-up: 2d modelisation," in *Tribology Series* (M. P. D. Dowson, G. Dalmaz and A.A Lubrecht, ed.), vol. Volume 41, pp. 477–488, Elsevier, 2003.
- [134] Y. Qiu and M. M. Khonsari, "Performance analysis of full-film textured surfaces with consideration of roughness effects," *Journal of Tribology*, vol. 133, no. 2, p. 021704, 2011.
- [135] S. Timoshenko, S. Woinowsky-Krieger, and S. a. v. U. s. a. architektu?ry, *Theory of Plates and Shells*. N. Y. : Mcgraw-hill, 2nd ed ed., 1959. The conference was organized by the Institute of Construction and Architecture of Slovak Academy of Sciences, Bratislava.
- [136] C. H. Yao, D. L. Feke, K. M. Robinson, and S. Meikle, "Modeling of chemical mechanical polishing processes using a discretized geometry approach," *Journal of the Electrochemical Society*, vol. 147, pp. 1502–1512, Apr. 2000. WOS:000086343800045.
- [137] G. S. Grover, H. Liang, S. Ganeshkumar, and W. Fortino, "Effect of slurry viscosity modification on oxide and tungsten CMP," *Wear*, vol. 214, pp. 10–13, Jan. 1998.
- [138] C. F. Higgs III, S. H. Ng, L. Borucki, I. Yoon, and S. Danyluk, "A Mixed-Lubrication Approach to Predicting CMP Fluid Pressure Modeling and Ex-

- periments,” *Journal of The Electrochemical Society*, vol. 152, no. 3, p. G193, 2005.
- [139] D. Zhao, Y. He, and X. Lu, “In Situ Measurement of Fluid Pressure at the Wafer-Pad Interface during Chemical Mechanical Polishing of 12-inch Wafer,” *Journal of The Electrochemical Society*, vol. 159, pp. H22–H28, Jan. 2011.
- [140] D. White, D. Boning, and A. Gower, “Characterization of endpoint and wafer level nonuniformity using in situ thermography,” in *Proceedings of the Fifth International Chemical-Mechanical Planarization for ULSI Multilevel Interconnection Conference (CMP-MIC)*, pp. 229–236, 2000.
- [141] P. Renteln and T. Ninh, “An Exploration of the Copper CMP Removal Mechanism,” in *Symposium P Chemical-Mechanical Polishing-Fundamentals and Challenges*, vol. 566 of *MRS Online Proceedings Library*, 1999.
- [142] H. Hocheng and Y.-L. Huang, “In Situ Endpoint Detection by Pad Temperature in Chemical–Mechanical Polishing of Copper Overlay,” *IEEE Transactions on Semiconductor Manufacturing*, vol. 17, pp. 180–187, May 2004.
- [143] S. Oh and J. Seok, “Modeling of chemicalmechanical polishing considering thermal coupling effects,” *Microelectronic Engineering*, vol. 85, pp. 2191–2201, Nov. 2008.
- [144] G. Srivastava and C. . F. I. Higgs, “A Fast, Experimentally validated, Particle Augmented Mixed Lubrication Framework to Predict CMP,” *MRS Online Proceedings Library*, vol. 1560, pp. null–null, 2013.

- [145] H. Blok, "The flash temperature concept," *Wear*, vol. 6, pp. 483–494, Nov. 1963.
- [146] H. J. Kim, P. Ehret, D. Dowson, and C. M. Taylor, "Thermal elastohydrodynamic analysis of circular contacts Part 1: Newtonian model," *Proceedings of the Institution of Mechanical Engineers, Part J: Journal of Engineering Tribology*, vol. 215, pp. 339–352, Jan. 2001.