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Effect of Microscale Protrusions on Local Fluid Flow and Mass Transport in the Presence of Forced Convection

Gerhard W. Matzen
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Ph.D. Thesis

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**Effect of Microscale Protrusions on Local Fluid Flow
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by

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Ph.D. Thesis

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MASTER

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Abstract
Effect of Microscale Protrusions
on Local Fluid Flow
and Mass Transport
in the Presence of Forced Convection

by
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1. Three-dimensional creeping flow around single, axisymmetric protrusions is studied numerically using the boundary-integral technique. Emphasis is placed upon cylindrical protrusions on plane walls for various height-to-radius (h -to- a) aspect ratios, but cones and sections of spheres protruding from plane walls are also briefly examined. The presented items include shear-stress distributions, shear-stress contours, extents of the fluid-flow disturbance, total forces and torques on the cylinders, streamlines, and skin-friction lines. Also included is a discussion of flow topology around axisymmetric geometries.

No flow reversal is observed for cylindrical protrusions with aspect ratios greater than 2.4 to 2.6. At higher aspect ratios, the fluid tends to be swept around cylindrical protrusions with little vertical motion. At lower aspect ratios, the strength of the recirculation increases, and the recirculation region becomes wider in the transverse direction and narrower in the flow direction. Also, the recirculation pattern begins to resemble the closed streamline patterns in two-dimensional flow over square ridges. However, unlike two-dimensional flow, closed streamline patterns are not observed.

For arbitrary axisymmetric geometries, the extent of the fluid-flow disturbance can be estimated with the total force that is exerted on the protrusion. When the same force is exerted on protrusions with different aspect ratios, the protrusion with the higher aspect ratio tends to have a greater disturbance in the flow direction and a smaller disturbance in the transverse direction. The total force exerted on cylindrical protrusions with rounded corners is only slightly lower than the total force exerted on cylindrical protrusions with sharp corners.

2. Mass transfer around insulating, cylindrical protrusions on an electrode surface is studied both numerically and experimentally, and good agreement is obtained between the two. For the numerical work, a commercially available finite-element program is used, and only a single, insulating protrusion is examined in laminar flow ($0.56 < Re_p < 5$), where $Re_p = \beta h^2 / \nu$, β is the shear rate at the wall, ν is the kinematic viscosity, and h is the protrusion height. For the experiments, the limiting-current technique is used to measure local mass-transport rates associated with the reduction of $Fe^{3+} + e^- \rightarrow Fe^{2+}$ around a $\sim 50 \mu m$ tall and $\sim 90 \mu m$ diameter single, isolated cylindrical protrusion, embedded into a planer platinum surface, as well as when such a protrusion is surrounded by an array of similar cylinders. The measurements involve 0.025 M $Fe_2(SO_4)_3$ and 0.05 M $FeSO_4$ solutions ($Sc \sim 1600$), in both laminar ($0.56 < Re_p < 3.64$) and turbulent ($13 < Re_p < 127$) regimes. The counterelectrode is placed 0.3175 cm away from the working electrodes in the opposite channel wall.

The measurements are obtained on a segmented electrode that we designed and constructed in the Microfabrication Laboratory on the Berkeley campus using a thermally oxidized 100 mm silicon wafer as a substrate. The working electrodes consist of $22, 48.5 \mu m \times 48.5 \mu m$ square platinum microelectrodes embedded within, but electrically isolated from, a $5 mm \times 5 mm$ square platinum "buffer" electrode. The current is collected by individual aluminum lines that are connected to the electrodes through contact holes in a silicon-dioxide layer. The protrusions are constructed using photosensitive polyimide. For the protrusion-array experiments, the array repeats 6 times upstream and downstream of the central protrusion and 2.5 times to either side of the central protrusion. For the protrusion-array or the single-protrusion experiments, the microelectrodes are arranged in a cross pattern around the central protrusion or the single protrusion, respectively.

Both the experimental and numerical findings suggest that the wake region is the least favorable for mass transport, except for the experiments at $Re_p > \sim 50$ for a single, insulating protrusion. For this exception, the mass flux 2.41 cylinder radii (r_{cyl}) upstream from the center of the protrusion is comparable to the mass flux between ~ 5 and $\sim 9 r_{cyl}$ downstream from the center of the protrusion. At similar Reynolds numbers for a protrusion array, the mass flux is more favorable in front of the protrusion than downstream of the protrusion by a factor of about 1.5.

The numerical results at $0.56 < Re_p < 5$ suggest that the single protrusion redistributes the reaction instead of increasing or decreasing the total mass flux to the electrode.

That is, regions of enhanced mass transport appear to balance regions of diminished mass transport so that the the total mass flux is the same with or without the single protrusion. Over a large area around the protrusion, mass transport is impeded because the shear stress at the electrode surface is attenuated compared to its undisturbed value far from the protrusion. Immediately in front of the protrusion, mass transport is enhanced owing to convection toward the electrode, and, immediately behind the protrusion, mass transport is diminished owing to convection away from the electrode. In addition to the enhancement in front of the protrusion, the diminished mass transport around the protrusion is also balanced by a slight mass-transport enhancement farther downstream of the protrusion.

To my parents

 

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Special thanks to my committee members—John Newman, Rolf Muller, Kim Kinoshita, and James Evans—for reading my thesis and providing many insightful comments.

When I first started this project, I did not have the first idea how to approach it, either numerically or experimentally. The numerical work seemed unapproachable without commercially available software because of the three-dimensional nature of the problem. The experiments were difficult because of the scale of the protrusions that were required.

I first made inroads with the numerical work when I stumbled across the book *Boundary Integral and Singularity Methods for Linearized Viscous Flow* by Professor Costas Pozrikidis. From his book, I realized that the fluid-flow problem was tractable. Then, with considerable help from Professors Newman and Pozrikidis, I finally understood the boundary-integral technique.

The experiments remained troublesome. Years of frustration would follow until a suggestion—the suggestion, he had many good ones—from David Hebert changed everything. Afterwards, I knew the experiments could be done.

Along the way, I warmed to the idea of using the commercial software package called FIDAP for the mass transport problem. Greg Mulhern welcomed FIDAP to Mordor (the aptly named computer in the Soane lab) and provided technical support. Greg did not know what was coming, but he remained supportive. Greg also worked with me in the Berkeley Microlab. He was my sounding board for ideas.

During the dark years, when progress seemed impossible, I found solace with my

friends. I started hanging with Greg Mulhern and Steve Lambert, and we became a trio. I went on many biking trips with Greg. During one of the longer rides, Greg was inspired to say: "I feel like I have one muscle in my body...and it is sore," which I still quote to this day. Steve was always next door to the Tobias lab, keeping a silent vigil over his computer. From my TA assignments, I met a number of other friends: Pedro Corneo, Dave Frey, Shaun Luper, Juleh Minoo, Diana Whittier, *etc.* Shaun told me that my gravestone should be a large, flat granite slab with a single protrusion on top. Through this group, I met Eric Wingfield, whose company I still enjoy while sea kayaking. I had many good experiences with this bunch including the legendary seminal Angel Island camping trip, fourth of July picnics, and Wild Turkey parties.

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Chapter 1

Introduction

1.1 Motivation, scope, brief conclusions, and related literature

This thesis addresses the problem of fluid flow and mass transport around small protrusions in the presence of flowing electrolyte. The topic was motivated by the phenomenon of striation formation during zinc electrodeposition in the presence of forced convection. Zinc striations consist of ridges of zinc oriented parallel to the direction of the streamlines near the electrode surface. Under a wide variety of experimental conditions, zinc striations evolve from initial growth centers, or nuclei, randomly positioned on the substrate. Zinc is deposited preferentially in the wake of these nuclei (although preferential deposition occurs in front of the nuclei to a lesser degree) until the individual nuclei connect into ridges to form striations. Zinc nuclei are shown in Figure 1.1. The figure, taken from Tsuda's master's thesis [1], shows a sequence of four photographs at different deposition times over a small portion of a rotating disk electrode. After 18 minutes of deposition, the nuclei are noticeably elongated in the direction of flow. An example of a fully striated deposit on a rotating disk electrode, taken from Faltemier's thesis [2], is shown in Figure 1.2. The striations are parallel to the streamlines near the surface of the rotating disk electrode.

Striated metal deposits are discussed in more detail in Section 1.2.

Commonly, it is suggested that localized mixing around the initial growth centers causes enhanced mass transport in the wake and, as a result, preferential deposition in this region. There are a few troubling aspects to this explanation that are addressed in this thesis:

1. Preferential deposition behind the nuclei begins when the nuclei are between, approximately, 1 and 20 μm in height. A Reynolds number based on the height of these protrusions will be small, and mixing effects are not expected to be large.
2. The suggestion that local mixing causes enhanced mass transport in the wake is made with limited knowledge about the nature of fluid mixing behind protrusions at low Reynolds numbers.
3. If mixing effects are expected to be small, is mass transport really expected to be favorable in the wake region?

The first item is addressed in this chapter. The second item is addressed in Chapter 2. In that chapter, creeping flow around single, cylindrical protrusions of various aspect ratios is modeled using the boundary integral technique. The computer code was written in this laboratory. Although cylindrical protrusions receive the most emphasis, some comparisons are made to sections of spheres and cones protruding from a plane wall. It is found that a recirculation region can, indeed, exist even around infinitesimally small protrusions, but the streamline trajectories would not favor mass transport to the wake region. The third item is addressed in Chapter 4. In that chapter, experimental and numerical mass-transfer results suggest that the wake region is the least favorable region for mass transport. The limiting-current technique [3] is used for the experiments, and a commercially available finite element program called FIDAP (Fluid Dynamics International, Inc.) is used for the numerical work (the boundary-integral technique could not be used to treat the mass transport). Single, insulating cylindrical protrusions and an array of insulating cylinders

Figure 1.1: Pictures from Tsuda's thesis [1] of nodular Zinc growth at short deposition times on a small portion of a rotating disk electrode: (A) 3 minutes, (B) 6 minutes, (C) 9 minutes, (D) 18 minutes. 10 mA/cm^2 , 800 RPM, 1 M ZnCl_2 . The flow direction is from the top left to the bottom right. XBB 817-6774A

Figure 1.2: An example of a fully striated zinc deposit on a rotating disk electrode from Faltemier's thesis [2] (30 mA/cm^2 , 40 minutes, 400 RPM, 1 M ZnCl_2 , $\text{pH}=2.4$). XBB 784-11239A

are used as the flow obstacles for the experiments. Note that the zinc reaction is NOT directly studied. A ferric-ferrous redox couple is used instead so that the working electrode geometry remains constant during an experiment. Finally, in Chapter 3, the experimental apparatus is described, and its characterization is discussed.

Our results do not support the contention that striations form as a result of enhanced mass transport of zinc in the wake region. In view of its intuitive appeal, however, it is not surprising that this explanation has been used, at least in part, by a number of researchers (for example page 96 in [1], page 61 in [4], and page 97 in [5]). Also, detailed measured or theoretical mass-transport distributions around small protrusions at low protrusion Reynolds numbers, which could have been used to discount the explanation *a priori*, appear to be unavailable in the literature.

Before the literature is discussed, a protrusion Reynolds number, Re_p , is defined so that we can define our range of interest. Re_p is defined to be

$$Re_p = \frac{\beta h^2}{\nu}, \quad (1.1)$$

where β is the undisturbed shear rate at the electrode, h is the height of the protrusion, and ν is the kinematic viscosity. Another protrusion Reynolds number, Re'_p , is defined as

$$Re'_p = \frac{V_{top} h}{\nu}, \quad (1.2)$$

where the velocity at the top of the protrusion, V_{top} , has replaced βh . Since the protrusions are small, the velocity profile will be approximately linear over the protrusion height, and Re_p will be nearly identical to Re'_p .

Tsuda [1] estimated $Re'_p=0.95$ for a $16 \mu\text{m}$ tall zinc nucleus located 7.25 cm from the center of a disk rotating at 800 RPM. Usually, a striation pattern is already visible before individual nuclei grow to a height of $16 \mu\text{m}$. Hence, the Reynolds number at which the nuclei begin to propagate into striations is on the order of 1 or less. However, in turbulent flow, where the shear rate at the surface is high, we estimate that protrusion Reynolds numbers on the order of 10 may occur. Faltmier [2] noted that striations grow more rapidly and are

more clearly defined at higher flow rates. To incorporate fully the effects of low and high flow rates, a Reynolds number range of $Re_p = 0.56$ to 127 was chosen for the experiments that are described in Chapter 5. The bulk fluid flow was laminar for $0.56 < Re_p < 3.64$ ($250 < Re < 1500$) and turbulent for $13 < Re_p < 127$ ($3200 < Re < 12000$), where Re is the Reynolds number based on the hydraulic diameter of the flow channel and the average fluid velocity. The Re_p for the numerical simulations ranged from 0.56 to 5.

The protrusion Reynolds numbers for the laminar flow experiments ($0.56 < Re_p < 3.64$) are far too small to induce turbulence. Instead, the onset of turbulence is governed by the usual stability criterion of $Re = 2000$. Below, a rough idea is given for the Re'_p sufficient to induce turbulence (transition Reynolds numbers) to show that the protrusions are, indeed, too small to cause this to happen. It is difficult to pin down hard numbers on transition Reynolds numbers since most of the data are for boundary-layer flows, where the transition to turbulence appears to be a function of boundary-layer thickness as well as Re'_p . Also, most of the data are for two-dimensional disturbances, such as a trip wire in a flow channel, instead of three-dimensional disturbances, such as a protrusion. It is generally agreed that, under otherwise identical conditions, flows are more stable to three-dimensional disturbances than to two dimensional disturbances (see review article by Sedney [6]). For a two-dimensional roughness element (circular wires in both cases below), Goldstein [7, see Schlichting p. 537] found no effect on the transition to turbulence for $Re_p \leq 49$.¹ The turbulent transition occurred downstream of the disturbance. Fage and Preston [7] found that turbulence originates at a two-dimensional disturbance for $Re_p = 400$.

In contrast to two dimensional disturbances, the transition for three-dimensional disturbances occurs at higher Reynolds numbers, and the turbulent region moves to the location of the roughness element over a narrow Reynolds number range. A transition Reynolds number of $Re'_p = 600$ is reported by Tani [8] for three-dimensional roughness elements (cylinders or spheres, height to diameter ratio of 1). This upper limit could be disputed, however, since Baker observed stable laminar flows at much higher protrusion

¹The actual reported value is $Re_p^* \leq 7$, but this Reynolds number is related to Re_p by $Re_p^* = \sqrt{Re_p}$.

Reynolds numbers (for a cylinder with a height to diameter ratio of 0.5 [9]). Nevertheless, it is clear that the protrusions in our experiments and the size of the zinc nuclei that appear before striations are formed are too small to induce turbulence.

Next, the literature relevant to mass or heat transfer distributions around protrusions is discussed. The vast body of information concerning the overall increase in mass or heat transfer to rough surfaces is not considered.

Rogers and Taylor [10] studied the effect of small protrusions on mass transport to a rotating disk. When coumarin was added to a Watts-type nickel plating solution, a striated nickel deposit formed. Smaller protrusions ($\sim 10 \mu\text{m}$ tall) created the most well-defined striations, and the Re'_p of these smaller protrusions was on the order of 1 (the value of 6 that they report must be in error). The protrusions, or burrs, had sharp corners because they were produced by depressing a sharp probe tip into the surface of the electrode. Experiments were performed using coumarin labeled with carbon-14. Conditions were chosen so that the reduction of coumarin was mass-transport limited. From autoradiographs, they determined that mass transport of coumarin was enhanced to the protrusions and diminished in the wake. This result is in direct support of the findings of this investigation.

Carlson [11] studied mass transfer of copper around conducting cylindrical protrusions (0.1 mm to 1 mm in height) and around conducting and insulating spherical protrusions (1.3 mm diameter) in turbulent flow for, approximately, $20 < Re'_p < 1000$.² He determined that the deposit thickness was enhanced over a region extending about 4 protrusion radii upstream and extending about 40 protrusion radii downstream. He came to the general conclusion that deposition in the wake region was enhanced by a factor of 2. Immediately behind the protrusion, however, there appeared to be a region of low mass transport. Figure 1.3 shows typical deposits that he obtained. Enhanced mass transport in

²Carlson calculated a protrusion Reynolds number of 10 for his 0.1 mm tall protrusions based on the average velocity over the height of the protrusion. His 0.1 mm tall protrusion was entirely within the viscous sublayer. Hence, the velocity profile is linear, and the corresponding Re'_p should be 20. The upper limit of $Re'_p = 1000$ is our estimation for a 1 mm tall protrusion in turbulent channel flow at $Re = 50000$. The tip of the protrusion is in the turbulent core, and the velocity at the top of the protrusion was estimated using the universal velocity profile.

the wake region of single, insulating cylinders at $Re_p=69$ and 126 was also observed in this study, but significant enhancement is not observed at lower Reynolds numbers (Re_p of 5 or less).

Unfortunately, the above studies do not give detailed, quantitative mass-transport distributions around the protrusions, and this information is apparently unavailable in the literature over our Reynolds number range of interest. However, at significantly higher Reynolds numbers (Reynolds numbers of 4000 to 1.3×10^5 based on the protrusion diameter and the free-stream velocity), detailed heat-and mass-transport distributions have been measured around single and multiple cylindrical protrusions for turbulent boundary-layer flows in air streams. The interested reader is referred to Goldstein, Chyu, and Hain [12] (single cylinder, $Re=4000$), Chyu and Goldstein [13] (in-line and staggered cylindrical protrusion arrays, $Re=1.68 \times 10^4$), and Fisher and Eibeck [14] (single cylinder, $Re=7.7 \times 10^4$ to 1.3×10^5).

1.2 Striated metal deposits

Striated metal deposits have been observed in various metals under a wide range of deposition conditions. Copper [15–17], silver [18], and nickel [10, 19] exhibit striated deposits in the presence of additives. Zinc [1, 2, 4, 5, 17, 20–22] exhibits striated deposits even in ultrapure electrolytes [1] over a wide pH range (over at least $1.9 < pH < 5$ in acid electrolytes [2]). In all of the cases above, the striations appear over a finite current density range. Usually, the current densities in this range correspond to a region of the current *vs.* potential curves where the current is very sensitive to small changes in polarization. These sensitive regions appear for copper and nickel only in the presence of additives (no polarization curves were found for silver). Sometimes, negative polarization resistances are observed in the sensitive regions. That is, the current increases with decreased polarization, resulting in 'S-shaped' current *vs.* potential curves. Such polarization curves have been observed by a number of investigators [23–25, 17] and have been theoretically calculated

$$Re = 23,000; i/i_L = 1.0$$

Figure 1.3: Copper deposits around conducting spheres, nonconducting spheres, and conducting cylinders [11]. (a-left) insulating sphere $D=1.30$ mm; (b-left) conducting sphere $D=1.30$ mm; (c-left) conducting cylinder $D=0.65$ mm, $h=1.00$ mm; (a-right) insulating sphere $D=0.62$ mm; (b-right) conducting cylinder $D=0.31$ mm, $h=0.50$ mm; (c-right) conducting cylinder $D=0.31$ mm, $h=1.00$ mm. The acrylic coating did not completely cover the nonconducting spheres resulting in a spotty deposit.

by Epelboin *et al.* [23]. Lee and Jorné [26] later improved Epelboin's model by correctly accounting for vacancy sites. Another common feature between the different metals is that the kinetics tend to decrease with increasing additive concentration in the case of copper [16,18] and nickel [19] and increasing hydrogen ion concentration (in acid electrolytes) [27,26] in the case of zinc.

In the remainder of this section, the discussion is limited to zinc-striation formation in acidic electrolytes. In the initial stages of zinc deposition on platinum, the surface is covered by a thin layer of zinc, zinc nuclei form, and the nuclei begin to grow [4]. After certain nuclei reach a critical height (between 1 and 20 μm), they begin to elongate in the direction of flow, consuming smaller nuclei in the process. At any given current density, the critical height decreases with Reynolds number. However, the nuclei are always smaller and more numerous at higher current densities. Using *in-situ* video microscopy, Mc Vay [4] determined that zinc is deposited preferentially in the wake of the nuclei, although the deposit still forms upstream and to the sides of the nuclei to lesser degrees. Eventually, the individual nuclei connect, and a fully striated deposit results.

Zinc striations form well below the limiting current (for example, between 10 and 40 mA/cm^2 in ZnSO_4 electrolytes and between 15 and 70 mA/cm^2 in ZnCl_2 electrolytes [5]). At higher current densities, where mass-transfer effects become more important, the striations disappear, and a flat deposit forms instead. This indicates that striations result from a combination of mass transport and kinetic effects. The frequency of the striations (*i.e.*, the number of striations per unit length) increases with current density, and the frequency at any given current density depends on the substrate. The frequency is largely unaffected by flow rate, pH, anion, or the concentration of zinc ions, although Yee and Jorné [21] found that the striation frequency was affected by ZnSO_4 concentration in an inconclusive and complicated way. Striations are formed in noncomplexing (ZnSO_4) as well as complexing (ZnCl_2 , ZnBr_2) electrolytes. Buoyancy effects are not important because striations appear on downward-facing and upward-facing electrodes [17]. Zinc deposition is accompanied by hydrogen evolution because the open-circuit potential of zinc is -0.763 V

vs. the standard hydrogen electrode. However, hydrogen is typically evolved at low levels because the exchange current density for hydrogen reacting on zinc is very low [28]. Mc Vay found that striations formed even when the current efficiency was between 98 and 100% [4].

Of the factors listed above, the critical height at which nuclei begin to elongate into striations and the S-shaped polarization curves are of most interest for this study. At the critical height, it is unlikely that vortices suddenly form because vortices can occur even for infinitesimal protrusion heights (see discussion in Chapter 2). It seems more likely that the critical height is related to high Péclet numbers rather than high Reynolds numbers. While Re_p increases from 0 to 1, the Péclet number ($Pe_p = Re_p Sc$) increases from 0 to values on the order of 1000. In other words, it is suggested that convection rapidly dominates over diffusion for very small nuclei, at which point pre-existing flow patterns begin to influence the mass transport. Once this occurs, the zinc nuclei begin to elongate in the direction of flow by some poorly understood mechanism.

The S-shaped kinetics is discussed at the end of Chapter 4, where it is used to suggest a possible mechanism for striation formation based on the mass-transfer distributions that we obtain. Here, we only mention that the current-density range for which zinc striations are observed is larger than the current-density range for which negative polarization resistances are observed [17]. The fact that negative polarization resistances are not universally required for striations to form is disconcerting since it would be convenient to point to this feature of the kinetics as being essential. A possible explanation for this may lie in the heterogeneous nature of the electrode surface. For example, Sutija [5, page 97] suggested an exchange current density for the zinc reaction of 100 mA/cm² on the nucleated growth centers and 1 mA/cm² on the surrounding electrode surface. It could be that the surrounding surface is in the negative polarization regime while the nuclei themselves are well outside of it.

Chapter 2

Modeling Three-dimensional Creeping Flow around Arbitrary, Axisymmetric Protrusions using the Boundary-Integral Technique

2.1 Introduction

It is commonly hypothesized that zinc striations form as a result of localized mass-transport enhancement by “fluid mixing” in the wake of zinc nuclei. However, zinc striations occur even when the Reynolds number (based on the protrusion height) is on the order of 1, where the creeping-flow assumption ($Re_p=0$) is reasonable. Hence, to a first approximation one would expect any mixing (whatever this mixing may be) to be antisymmetric on either side of the protrusion. In other words, if the streamlines in a vortex circulate in the clockwise direction on one side of the protrusion, the corresponding antisymmetric vortex will rotate in the counterclockwise direction on the opposite side of the protrusion. It is possible that antisymmetric mixing could cause mass-transport enhancement on one side of the protrusion

but not the other, but choosing the wake region ahead of time without knowledge of the fluid flow may not be appropriate.

As a first attempt at elucidating the nature of the fluid flow, we study the three-dimensional fluid motion resulting from a linear infinite shear flow over single axisymmetric protrusion geometries in the limit of creeping flow using the boundary-integral technique. Specifically, we shall focus on cylindrical protrusion geometries, but we briefly examine other geometries including hemispherical and conical protrusions. For a general description of the boundary-integral technique as applied to viscous flow, the reader is referred to Pozrikidis [29]. Pozrikidis outlines the procedure for solving three-dimensional flow problems around axisymmetric geometries, and the final integral equations that we use can be found in his book. A more detailed derivation is presented here because only axisymmetric protrusions are discussed. Also, the approach used in this study to reduce the dimensionality of the integral equations from a two-dimensional surface integral to a one-dimensional line integral is less general than in [29] but perhaps easier to understand. The sensitivity of the numerical calculations to mesh density is tested in Appendix A.8.

There have been surprisingly few papers published on creeping flow over axisymmetric protrusion geometries. To our knowledge, O'Neill [30] was first to solve the Navier-Stokes equations correctly for an axisymmetric protrusion on a plane wall. He formulated a solution for linear shear flow over a sphere in contact with a plane using tangent-sphere coordinates, and he calculated the total force and torque on the sphere. Also, he pointed out that the total force on the sphere is equal and opposite to the disturbance force on the wall. For arbitrary protrusion shapes, it will be shown that the total force is related to the disturbance force on the wall but the forces are not always equal and opposite. This result will be used to show that the extent of the flow disturbance by a protrusion (as determined by the relaxation of the shear stress on the wall to its value at infinity) can be predicted with only the total force on the protrusion.

Over 10 years later, Price [31] used expansions in spherical polar coordinates to formulate a solution for linear shear flow over a hemispherical bump. The force and torque

on the hemisphere were calculated, and one point of zero shear stress (or a singular point) on the protrusion and one point of zero shear stress on the wall were determined. Price correctly interpreted the singular point on the protrusion as a point of separation (*i.e.*, it is a point of separation in the wake of the protrusion) and the singular point on the wall as a point of attachment, but he mistakenly concluded that there is a streamline connecting the two points. We provide the correct streamline pattern for the hemispherical protrusion for comparison with the streamline pattern for cylindrical protrusions near the end of this chapter.

Recently, Pozrikidis [32] used the boundary-integral technique to solve for linear shear flow over arbitrary axisymmetric protrusions; this is the same technique used in this chapter. However, Pozrikidis focuses on protrusions which are sections of spheres and spheroidal protrusions whereas we concentrate on cylindrical protrusions. He presents streamline patterns and shear-stress distributions, and he calculates the total force and torque for his geometries. We present the corresponding plots and tables for our cylindrical geometries.

We should note that Pozrikidis used a slightly different formulation from ours. Specifically, he did not eliminate the double-layer integral, which is needed for the most general procedure but not specifically for axisymmetric protrusions. Also, we implement the wall Green's function whereas he does not. This allows us to resolve vortices near the wall and to accurately calculate the extent of the flow disturbance without using an excessive number of nodes.

2.2 Basic equations

The Lorentz reciprocal relation [29] is a convenient starting place to derive the boundary integral equations. The relation is

$$\frac{\partial}{\partial x_k} (u'_i \sigma_{ik} - u_i \sigma'_{ik}) = 0 \quad (2.1)$$

where u'_i and u_i are two velocity distributions and σ'_{ik} and σ_{ik} are the corresponding stress tensors. The equation applies as long as u'_i and u_i are regular flows (*i.e.*, the fluid velocity does not go to infinity at any point). The indices i , j , and k correspond to the Cartesian coordinates x , y , and z , respectively, and a repeated subscript implies summation over this range (standard Einstein notation). In the following, bold-face text indicates a vector quantity (*e.g.*, $\mathbf{x} = x_i$). The Lorentz reciprocal relation is derived in Appendix A.1.

It is useful to let u_i and σ_{ik} represent the general flow field and for u'_i and σ'_{ik} to correspond to the flow field due to a point force. Thus, u'_i and σ'_{ik} can be written in the form

$$u'_i(\mathbf{x}) = \frac{1}{8\pi\mu} G_{ij}(\mathbf{x}, \mathbf{x}_0) g_j \quad \sigma'_{ik}(\mathbf{x}) = \frac{1}{8\pi} T_{ijk}(\mathbf{x}, \mathbf{x}_0) g_j \quad (2.2)$$

where g_j is a point force located at $\mathbf{x}_0$ and μ is the viscosity. Physically, u'_i is the velocity at some observation point $\mathbf{x}$ resulting from a point force at the pole $\mathbf{x}_0$. G_{ij} is referred to as the Green's function for creeping flow. Other common names are the fundamental solution or propagator. The Green's function can assume different forms depending upon the boundary conditions for u'_i . $T_{ijk}(\mathbf{x}, \mathbf{x}_0)$ is the stress tensor associated with G_{ij} .

If g_i is taken to be a point force in an unbounded medium, the corresponding fundamental solution is called the free-space Green's function (G_{ij}^F) or the Stokeslet. The corresponding velocity profile is identical to the velocity profile for an infinitesimally small sphere flowing through a liquid that has no boundaries. The equations for the free-space Green's function and its associated stress tensor T_{ijk}^F are

$$G_{ij}^F(\mathbf{x}, \mathbf{x}_0) = \frac{\delta_{ij}}{r} + \frac{\hat{x}_i \hat{x}_j}{r^3} \quad T_{ijk}^F(\mathbf{x}, \mathbf{x}_0) = -6 \frac{\hat{x}_i \hat{x}_j \hat{x}_k}{r^5} \quad (2.3)$$

where x_i are in Cartesian coordinates ($x_i = (x_1, x_2, x_3) = (x, y, z)$), $\hat{\mathbf{x}} = \mathbf{x} - \mathbf{x}_0$, and $r = |\hat{\mathbf{x}}|$. Note that G_{ij}^F is infinite when $\mathbf{x} = \mathbf{x}_0$. As a result, u'_i is also infinite at $\mathbf{x}_0$ and the flow is not regular at this point. Equation 2.1 is still valid, however, as long as one considers a domain in which $\mathbf{x}_0$ is excluded. The free-space Green's function shall be used for determining shear-stress distributions.

Figure 2.1: An example control volume.

Sometimes it is convenient to use different Green's functions which are identically equal to zero on certain boundaries of the domain. Specifically, we shall employ the Green's function for a plane wall (G_{ij}^w) for calculating streamlines and for calculating shear stresses when very accurate values are needed. The wall Green's function is the solution to the Navier-Stokes equations for a point force in the vicinity of a plane wall. If the wall is located at $x = x_w$, parallel to the yz -plane, then

$$G_{ij}^w(x = x_w, y, z; \mathbf{x}_0) = 0. \quad (2.4)$$

As the pole $\mathbf{x}_0$ is approached, the wall Green's function behaves like the free-space Green's function to leading order, and the associated velocities approach infinity. The equations for the wall Green's function are given in Appendix A.5.

Substituting equation 2.2 into equation 2.1 and discarding the arbitrary constant g_j , one obtains

$$\frac{\partial}{\partial x_k} [G_{ij}(\mathbf{x}, \mathbf{x}_0) \sigma_{ik}(\mathbf{x}) - \mu u_i(\mathbf{x}) T_{ijk}(\mathbf{x}, \mathbf{x}_0)] = 0. \quad (2.5)$$

Now consider the control volume, V , shown in Figure 2.1. The volume is bounded by the external and internal surfaces D . The normal vector, $\mathbf{n}$, points toward the interior of the domain, and $\mathbf{x}_0$ lies outside of the domain. Integrating equation 2.5 over V and

applying the divergence theorem, one obtains

$$\int_D [G_{ij}(\mathbf{x}, \mathbf{x}_0) \sigma_{ik}(\mathbf{x}) - \mu u_i(\mathbf{x}) T_{ijk}(\mathbf{x}, \mathbf{x}_0)] n_k(\mathbf{x}) dS(\mathbf{x}) = 0. \quad (2.6)$$

If $\mathbf{x}_0$ is moved inside the control volume, then the flow is no longer regular over the entire domain and equation 2.6 no longer applies. However, one can exclude $\mathbf{x}_0$ from the domain artificially by placing it inside an additional control volume V' . If the boundary of V' is taken to be an additional internal surface of the original control volume, then the divergence theorem can be applied once again. Next, one shrinks V' to an infinitesimal size. The result is that the right side of equation 2.6 is no longer zero. For the details of this exercise, the interested reader is referred to Pozrikidis [29, page 25]. The final equations are

$$\begin{aligned} - \int_D G_{ij}(\mathbf{x}, \mathbf{x}_0) \sigma_{ik}(\mathbf{x}) n_k(\mathbf{x}) dS(\mathbf{x}) \\ + \int_D \mu u_i(\mathbf{x}) T_{ijk}(\mathbf{x}, \mathbf{x}_0) n_k(\mathbf{x}) dS(\mathbf{x}) = \begin{bmatrix} 8\pi \\ 4\pi \\ 0 \end{bmatrix} u_j(\mathbf{x}_0) \quad (2.7) \end{aligned}$$

where the right side is $8\pi u_j(\mathbf{x}_0)$ for $\mathbf{x}_0$ located inside the control volume, $4\pi u_j(\mathbf{x}_0)$ for $\mathbf{x}_0$ located on the surface D , and 0 for $\mathbf{x}_0$ located outside the control volume. Also, $u_j(\mathbf{x}_0)$ is the velocity at the pole $\mathbf{x}_0$. The integral containing $G_{ij}(\mathbf{x}, \mathbf{x}_0)$ is known as the single-layer integral, and the integral containing $T_{ijk}(\mathbf{x}, \mathbf{x}_0)$ is known as the double-layer integral.

2.3 Elimination of the double-layer integral from the boundary-integral equations for flow over a protrusion

For flow over a protrusion on a plane wall, equations 2.7 can be simplified by eliminating the double-layer integral. This requires two hypothetical flows, one sharing the same domain as the actual flow, the other being external to the actual flow domain. No restrictions are placed upon the geometry of the protrusion. Consider the control volume in Figure 2.2. The actual flow and hypothetical flow 1 are bounded by the surface of the

Figure 2.2: The control volume around a protrusion on a plane wall.

protrusion, D_p , the wall, D_w , and a surface infinitely far away from the protrusion, D_i . Hypothetical flow 2 is bounded by D_b (which is coplanar to D_w) and D_p . The normal vectors associated with each surface are drawn in Figure 2.2. In the equations below, the normal vector n_k is equal to $\mathbf{n}_b$ on surface D_b , $\mathbf{n}_w$ on surface D_w , and so on.

Equation 2.7 is first applied to the actual flow. The double-layer integrals over D_p and D_w can be eliminated immediately because the velocity is zero over these surfaces. Over D_i , the velocity is equal to u_i^∞ , the undisturbed velocity distribution far from the protrusion. For the single layer integral, it is convenient to distinguish between the shear stress on D_p and D_w , σ_{ik} , and the shear stress on D_i , σ_{ik}^∞ . Equation 2.7 then becomes

$$\begin{aligned}
 - \int_{D_1, D_w} G_{ij}(\mathbf{x}, \mathbf{x}_0) \sigma_{ik}(\mathbf{x}) n_k(\mathbf{x}) dS(\mathbf{x}) - \int_{D_i} G_{ij}(\mathbf{x}, \mathbf{x}_0) \sigma_{ik}^\infty(\mathbf{x}) n_k(\mathbf{x}) dS(\mathbf{x}) \\
 + \int_{D_i} \mu u_i^\infty(\mathbf{x}) T_{ijk}(\mathbf{x}, \mathbf{x}_0) n_k(\mathbf{x}) dS(\mathbf{x}) = \begin{bmatrix} 8\pi \\ 4\pi \end{bmatrix} u_j(\mathbf{x}_0) \quad (2.8)
 \end{aligned}$$

where the right side of 2.8 is equal to 8π when $\mathbf{x}_0$ is located within the domain and 4π when

it is located on the boundary of the domain.

Equation 2.7 now is applied to hypothetical flow 1. The velocity and shear stress for this flow are set equal to u_i^∞ and σ_{ik}^∞ everywhere in the domain, including the boundaries D_p , D_i , and D_w . However, u_i^∞ is equal to 0 on D_w . Equations 2.7 then becomes

$$- \int_{D_p, D_w, D_i} G_{ij}(\mathbf{x}, \mathbf{x}_0) \sigma_{ik}^\infty(\mathbf{x}) n_k(\mathbf{x}) dS(\mathbf{x}) + \int_{D_p, D_i} \mu u_i^\infty(\mathbf{x}) T_{ijk}(\mathbf{x}, \mathbf{x}_0) n_k(\mathbf{x}) dS(\mathbf{x}) = \begin{bmatrix} 8\pi \\ 4\pi \end{bmatrix} u_j^\infty(\mathbf{x}_0) \quad (2.9)$$

where the right side is equal to 8π when $\mathbf{x}_0$ is located within the domain and 4π when it is located on the boundary of the domain. When 2.9 is subtracted from 2.8, all of the integrals over D_i cancel resulting in

$$- \int_{D_1, D_w} G_{ij}(\mathbf{x}, \mathbf{x}_0) \sigma_{ik}^p(\mathbf{x}) n_k(\mathbf{x}) dS(\mathbf{x}) - \int_{D_p} \mu u_i^\infty(\mathbf{x}) T_{ijk}(\mathbf{x}, \mathbf{x}_0) n_k(\mathbf{x}) dS(\mathbf{x}) = \begin{bmatrix} 8\pi \\ 4\pi \end{bmatrix} u_j^p(\mathbf{x}_0) \quad (2.10)$$

In equation 2.10, $u_i^p = u_i - u_i^\infty$ is the disturbance velocity due to the presence of the protrusion and, similarly, $\sigma_{ik}^p = \sigma_{ik} - \sigma_{ik}^\infty$.

Finally, equation 2.7 is applied to hypothetical flow 2. As for hypothetical flow 1, the velocity and shear stress are set equal to u_i^∞ and σ_{ik}^∞ everywhere in the domain, including the boundaries. In this case, u_i^∞ is equal to 0 on D_b . Equation 2.7 then becomes

$$- \int_{D_p} G_{ij}(\mathbf{x}, \mathbf{x}_0) \sigma_{ik}^\infty(\mathbf{x}) (-n_k(\mathbf{x})) dS(\mathbf{x}) - \int_{D_b} G_{ij}(\mathbf{x}, \mathbf{x}_0) \sigma_{ik}^\infty(\mathbf{x}) n_k(\mathbf{x}) dS(\mathbf{x}) + \int_{D_p} u_i^\infty(\mathbf{x}) T_{ijk}(\mathbf{x}, \mathbf{x}_0) (-n_k(\mathbf{x})) dS(\mathbf{x}) = \begin{bmatrix} 0 \\ 4\pi \end{bmatrix} u_j^\infty(\mathbf{x}_0) \quad (2.11)$$

where the right side is equal to zero when $\mathbf{x}_0$ is located outside the external domain (*i.e.*, within the actual flow domain) and 4π when it is located on the boundary of the external domain. In equation 2.11, the normal vector for surface D_p is written as $(-n_k(\mathbf{x}))$ because the normal vector must point towards the interior of the external domain.

The double layer integrals are eliminated when 2.11 is subtracted from 2.10:

$$\begin{aligned}
 & - \int_{D_p} G_{ij}(\mathbf{x}, \mathbf{x}_0) \sigma_{ik}(\mathbf{x}) n_k(\mathbf{x}) dS(\mathbf{x}) - \int_{D_w} G_{ij}(\mathbf{x}, \mathbf{x}_0) \sigma_{ik}^p(\mathbf{x}) n_k(\mathbf{x}) dS(\mathbf{x}) \\
 & + \int_{D_b} G_{ij}(\mathbf{x}, \mathbf{x}_0) \sigma_{ik}^\infty(\mathbf{x}) n_k(\mathbf{x}) dS(\mathbf{x}) = \begin{bmatrix} 8\pi u_j^p(\mathbf{x}_0) \\ 4\pi[u_j^p(\mathbf{x}_0) - u_j^\infty(\mathbf{x}_0)] \end{bmatrix} \quad (2.12)
 \end{aligned}$$

where the right side is equal to the top quantity when $\mathbf{x}_0$ is located within the actual flow domain and the right side is equal to the bottom quantity when $\mathbf{x}_0$ is located on the boundary of the actual flow domain. When $\mathbf{x}_0$ is on the boundary, $u_j(\mathbf{x}_0) = 0$, $4\pi[u_j^p(\mathbf{x}_0) - u_j^\infty(\mathbf{x}_0)] = -8\pi u_j^\infty(\mathbf{x}_0)$, and $8\pi u_j^p(\mathbf{x}_0) = -8\pi u_j^\infty(\mathbf{x}_0)$. Hence, the right side in 2.12 can be consolidated into a single term. Also, it is convenient to define a force vector, $f_i(\mathbf{x}) = \sigma_{ik}(\mathbf{x}) n_k$ to simplify the notation. Equation 2.12 then becomes

$$\begin{aligned}
 & - \int_{D_p} G_{ij}(\mathbf{x}, \mathbf{x}_0) f_i(\mathbf{x}) dS(\mathbf{x}) - \int_{D_w} G_{ij}(\mathbf{x}, \mathbf{x}_0) f_i^p(\mathbf{x}) dS(\mathbf{x}) \\
 & + \int_{D_b} G_{ij}(\mathbf{x}, \mathbf{x}_0) f_i^\infty(\mathbf{x}) dS(\mathbf{x}) = 8\pi \mu u_j^p(\mathbf{x}_0) \quad (2.13)
 \end{aligned}$$

Note that the integral over D_w can be truncated at some finite distance because $f_i^p(\mathbf{x})$ becomes vanishingly small far from the protrusion.

Finally, equation 2.13 can be written in the form

$$-8\pi \mu u_j^p(\mathbf{x}_0) = \int_C f_i(\mathbf{x}) G_{ij} dS(\mathbf{x}) \quad (2.14)$$

where C is a combination of the surfaces $D_p + D_w + D_b$. In equation 2.14, $f_i(\mathbf{x}) = f_i(\mathbf{x})$ on D_p , $f_i(\mathbf{x}) = f_i^p(\mathbf{x})$ on D_w , and $f_i(\mathbf{x}) = -f_i^\infty(\mathbf{x})$ on D_b . Also, $G_{ij}(\mathbf{x}, \mathbf{x}_0)$ has been written as G_{ij} to simplify the notation further. Note that when the wall Green's function is used, the integrals over D_w and D_b disappear. In addition, the integral equations for a protrusion on a plane wall are identical to the integral equations for a fixed obstacle above a plane wall when the wall Green's function is used. Since Goldman, Cox, and Brenner [33] calculated the total force and torque on a fixed sphere above a plane wall and since O'Neill [30] calculated the total force and torque on a sphere just touching a plane wall, their results can be used to check our numerical calculations. This is done in Appendix A.8.

Formula 2.14 gives 3 equations, one for each component of the disturbance velocity, $u_j^p(\mathbf{x}_0)$, and 6 unknowns, $u_j^p(\mathbf{x}_0)$ and $f_i(\mathbf{x})$. Equation 2.14 can be reduced to a set of 3 equations and 3 unknown functions by choosing the pole $\mathbf{x}_0$ to be on the flow boundaries where $u_j^p(\mathbf{x}_0)$ is equal to the known function $u_j^\infty(\mathbf{x}_0)$. Once the unknowns have been determined, equation 2.14 can be used to determine local velocities by moving the pole to locations within the domain.

2.4 The integral equations for axisymmetric geometries

In this section, the boundary integral equations are formulated for flow over an axisymmetric protrusion. A schematic of the problem is shown in Figure 2.3. In this figure, the cylindrical (x, σ, ϕ) and Cartesian (x, y, z) coordinate systems are superimposed on a cylindrical protrusion on a wall. The flow far from the protrusion is chosen to be

$$u_y^\infty(\mathbf{x}_0) = \kappa(x_0 - x_w) \bar{\mathbf{i}}_y \quad (2.15)$$

where κ is the shear rate in units of reciprocal time, x_w is the x -position of the wall (the wall is at $x_w = 0$ in Figure 2.3), x_0 is the x -position of the pole, and $\bar{\mathbf{i}}_y$ is a unit vector pointing in the y -direction. Although the protrusion is drawn as a cylinder in Figure 2.3, the analysis below holds for all axisymmetric protrusions (*i.e.*, hemispheres, cones, cylinders, *etc.*).

Although the fluid flow is three dimensional, the axisymmetric geometry and condition 2.15 allow the force components to be written as

$$\begin{aligned} f_x(x, \sigma, \phi) &= \cos(\phi) \mathfrak{F}_x(x, \sigma) \\ f_\sigma(x, \sigma, \phi) &= \cos(\phi) \mathfrak{F}_\sigma(x, \sigma) \\ f_\phi(x, \sigma, \phi) &= -\sin(\phi) \mathfrak{F}_\phi(x, \sigma) \end{aligned} \quad (2.16)$$

where $\mathfrak{F}_x$, $\mathfrak{F}_\sigma$, and $\mathfrak{F}_\phi$ are functions of x and σ only. These functional forms are deduced in Appendix A.2. The functional form of f_β^p is the same as f_β . To take advantage of 2.16, the appropriate boundary-integral equation, namely equation 2.14, must be transformed from

Figure 2.3: The coordinate system used for the boundary-integral solution.

Cartesian coordinates to cylindrical coordinates. The transformation is done generally; that is, it is not dependent upon equations 2.15 or 2.16.

For the transformation, the force components in Cartesian coordinates are related to the force components in cylindrical coordinates by

$$\begin{aligned} f_x(\mathbf{x}) &= f_x(\mathbf{x}) \\ f_y(\mathbf{x}) &= f_\sigma(\mathbf{x}) \cos(\phi) - f_\phi(\mathbf{x}) \sin(\phi) \\ f_z(\mathbf{x}) &= f_\sigma(\mathbf{x}) \sin(\phi) + f_\phi(\mathbf{x}) \cos(\phi) , \end{aligned} \quad (2.17)$$

and the velocity components in Cartesian coordinates are related to the velocity components in cylindrical coordinates by

$$\begin{aligned} u_x^v(\mathbf{x}_0) &= u_x^v(\mathbf{x}_0) \\ u_\sigma^v(\mathbf{x}_0) &= u_y^v(\mathbf{x}_0) \cos(\phi_0) + u_z^v(\mathbf{x}_0) \sin(\phi_0) \\ u_\phi^v(\mathbf{x}_0) &= -u_y^v(\mathbf{x}_0) \sin(\phi_0) + u_z^v(\mathbf{x}_0) \cos(\phi_0) . \end{aligned} \quad (2.18)$$

Substituting 2.17 into 2.14 and rearranging gives

$$\begin{aligned} -8\pi\mu u_j^v(\mathbf{x}_0) &= \int_C f_x(\mathbf{x}) G_{xj} dS(\mathbf{x}) + \int_C [\sin(\phi) G_{zj} + \cos(\phi) G_{yj}] f_\sigma(\mathbf{x}) dS(\mathbf{x}) \\ &\quad + \int_C [\cos(\phi) G_{zj} - \sin(\phi) G_{yj}] f_\phi(\mathbf{x}) dS(\mathbf{x}) \end{aligned} \quad (2.19)$$

where the subscript j is in Cartesian coordinates. Upon substituting 2.19 into 2.18 and rearranging, the resultant expression can be written in the form

$$-8\pi\mu u_\alpha^v(\mathbf{x}_0) = \int_C N_{\alpha\beta} f_\beta(\mathbf{x}) dS(\mathbf{x}) \quad (2.20)$$

where the indices $\alpha\beta$ run through (x, σ, ϕ) and $N_{\alpha\beta}$ is the Green's function in cylindrical

coordinates. $N_{\alpha\beta}$ is given by

$$\begin{aligned}
 N_{xx} &= G_{xx} \\
 N_{x\sigma} &= \sin(\phi)G_{zx} + \cos(\phi)G_{yx} \\
 N_{x\phi} &= \cos(\phi)G_{zx} - \sin(\phi)G_{yx} \\
 N_{\sigma x} &= \cos(\phi_0)G_{xy} - \sin(\phi_0)G_{xz} \\
 N_{\sigma\sigma} &= \cos(\phi_0)[G_{yy}\cos(\phi) + G_{zy}\sin(\phi)] + \sin(\phi_0)[G_{yz}\cos(\phi) + G_{zz}\sin(\phi)] \\
 N_{\sigma\phi} &= \cos(\phi_0)[-G_{yy}\sin(\phi) + G_{zy}\cos(\phi)] + \sin(\phi_0)[-G_{yz}\sin(\phi) + G_{zz}\cos(\phi)] \\
 N_{\phi x} &= -\sin(\phi_0)G_{xy} + \cos(\phi_0)G_{xz} \\
 N_{\phi\sigma} &= -\sin(\phi_0)[G_{yy}\cos(\phi) + G_{zy}\sin(\phi)] + \cos(\phi_0)[G_{yz}\cos(\phi) + G_{zz}\sin(\phi)] \\
 N_{\phi\phi} &= -\sin(\phi_0)[-G_{yy}\sin(\phi) + G_{zy}\cos(\phi)] + \cos(\phi_0)[-G_{yz}\sin(\phi) + G_{zz}\cos(\phi)]
 \end{aligned} \tag{2.21}$$

In 2.21, the Green's functions, G_{ij} , need to be written in cylindrical coordinates. For example, G_{yz} for the free-space Green's function (cf., equation 2.3) becomes

$$G_{yz}^F = \frac{\hat{y}\hat{z}}{r^3} = \frac{[\sigma\cos(\phi) - \sigma_0\cos(\phi_0)][\sigma\sin(\phi) - \sigma_0\sin(\phi_0)]}{r^3} \tag{2.22}$$

where

$$r = |\hat{\mathbf{x}}| = \sqrt{\hat{x}^2 + \sigma^2 + \sigma_0^2 - 2\sigma\sigma_0\cos(\hat{\phi})} \tag{2.23}$$

By making use of trigonometric identities and rearranging, the individual ϕ 's and ϕ_0 's in equation 2.21 can be written as the quantity $\hat{\phi} = (\phi - \phi_0)$. Although cumbersome, the transformations are straightforward. The final forms for $N_{\alpha\beta}$ are given in Appendix A.5 for both the free-space Green's function, G_{ij}^F , and the wall Green's function, G_{ij}^W .

Now that the transformation to cylindrical coordinates has been made, the general formulation given by 2.20 is applied to our specific problem. To do this, 2.20 is expanded to

$$-8\pi\mu u_\alpha^p(\mathbf{x}_0) + \int_{D_b} N_{\alpha\beta} f_\beta^\infty(\mathbf{x}) = \int_{D_p+D_w} N_{\alpha\beta} f_\beta(\mathbf{x}) dS(\mathbf{x}) . \tag{2.24}$$

The quantities on the left side of equation 2.24 are known from the boundary conditions as long as $\mathbf{x}_0$ is on the boundary. In cylindrical coordinates, the boundary conditions are

$$\begin{aligned} u_x^\infty(\mathbf{x}_0) &= 0 \\ u_\sigma^\infty(\mathbf{x}_0) &= \cos(\phi_0)\kappa(x_0 - x_w) \\ u_\phi^\infty(\mathbf{x}_0) &= -\sin(\phi_0)\kappa(x_0 - x_w) \end{aligned} \quad (2.25)$$

and

$$\begin{aligned} f_x^\infty(\mathbf{x}) &= 0 \\ f_\sigma^\infty(\mathbf{x}) &= \kappa\mu \cos(\phi) \\ f_\phi^\infty(\mathbf{x}) &= -\kappa\mu \sin(\phi) \end{aligned} \quad (2.26)$$

where pressure does not appear in equation 2.26 because the pressure was set to zero at infinity to stay consistent with 2.16 (see Appendix A.2).

Note that, unlike $N_{\alpha\beta}$, equations 2.16 and 2.26 are functions of ϕ instead of $\hat{\phi}$. By applying trigonometric identities, however, equations 2.16 and 2.26 can be re-written as

$$\begin{aligned} f_x &= [\cos(\phi_0)\cos(\hat{\phi}) - \sin(\phi_0)\sin(\hat{\phi})] \mathfrak{F}_x \\ f_\sigma &= [\cos(\phi_0)\cos(\hat{\phi}) - \sin(\phi_0)\sin(\hat{\phi})] \mathfrak{F}_\sigma \\ f_\phi &= [-\sin(\phi_0)\cos(\hat{\phi}) - \cos(\phi_0)\sin(\hat{\phi})] \mathfrak{F}_\phi \end{aligned} \quad (2.27)$$

$$\begin{aligned} f_x^\infty &= 0 \\ f_\sigma^\infty &= \kappa\mu [\cos(\phi_0)\cos(\hat{\phi}) - \sin(\phi_0)\sin(\hat{\phi})] \\ f_\phi^\infty &= \kappa\mu [-\sin(\phi_0)\cos(\hat{\phi}) - \cos(\phi_0)\sin(\hat{\phi})] \end{aligned} \quad (2.28)$$

Placing $\mathbf{x}_0$ on the protrusion or the wall so that $-u_\alpha^\nu(\mathbf{x}_0) = u_\alpha^\infty(\mathbf{x}_0)$, substituting

equations 2.25, 2.27, and 2.28 into 2.24, and writing $dS = \sigma d\phi dl = \sigma d\hat{\phi} dl$ finally leads to

$$\int_{(D_p+D_w)} \begin{bmatrix} Q_{xx} & Q_{x\sigma} & -Q'_{x\phi} \\ Q_{\sigma x} & Q_{\sigma\sigma} & -Q'_{\sigma\phi} \\ Q'_{\phi x} & Q'_{\phi\sigma} & Q_{\phi\phi} \end{bmatrix} \begin{bmatrix} \mathfrak{F}_x \\ \mathfrak{F}_\sigma \\ \mathfrak{F}_\phi \end{bmatrix} \sigma dl = \begin{bmatrix} \int_{(D_b)} [Q_{x\sigma} - Q'_{x\phi}] \kappa \mu \sigma dl \\ 8\pi\mu\kappa(x_0 - x_w) + \int_{(D_b)} [Q_{\sigma\sigma} - Q'_{\sigma\phi}] \kappa \mu \sigma dl \\ 8\pi\mu\kappa(x_0 - x_w) + \int_{(D_b)} [Q'_{\phi\sigma} + Q_{\phi\phi}] \kappa \mu \sigma dl \end{bmatrix} \quad (2.29)$$

where the integrals $Q_{\alpha\beta}$ and $Q'_{\alpha\beta}$ are given by¹

$$Q_{\alpha\beta}(\hat{x}, \sigma, \sigma_0) = \int_0^{2\pi} N_{\alpha\beta}(\hat{x}, \sigma, \sigma_0, \hat{\phi}) \cos(\hat{\phi}) d\hat{\phi} \quad (2.30)$$

$$Q'_{\alpha\beta}(\hat{x}, \sigma, \sigma_0) = \int_0^{2\pi} N_{\alpha\beta}(\hat{x}, \sigma, \sigma_0, \hat{\phi}) \sin(\hat{\phi}) d\hat{\phi} \quad (2.31)$$

In the matrix on the left side of equation 2.29, each position is occupied by a $Q_{\alpha\beta}$ or a $Q'_{\alpha\beta}$ but not both. That is, when $Q_{\alpha\beta}$ is nonzero at given $\alpha\beta$ position, the corresponding $Q'_{\alpha\beta}$ is zero and *vice versa*. Also, there are no $\sin(\phi_0)$ or $\cos(\phi_0)$ terms on either side of the equation because these terms cancel after the appropriate Q terms drop out. The “ $D_p + D_w$ ” terms were placed in parentheses to emphasize that the integral is now a line integral instead of a surface integral. When the integral is taken over (D_p) , $\mathfrak{F}_\beta$ is related to the actual force, f_β , through equations 2.16, and when the integral is taken over (D_w) , $\mathfrak{F}_\beta$ is related to the disturbance force, f_β^p , again through equations 2.16. The integrals given by equations 2.30 and 2.31 can be calculated efficiently. The calculation procedure is described in Appendix A.6. Finally, note that when the wall Green’s function is used, the integrals over (D_w) and (D_b) vanish because G_{ij}^w is identically equal to zero on these surfaces.

¹For the wall Green’s function, $Q_{\alpha\beta}$ and $Q'_{\alpha\beta}$ are functions of X in addition to $\hat{x}$, σ , σ_0 , and $\hat{\phi}$, where X is introduced in Appendix A.5.

2.5 Numerical calculations

The numerical evaluation of the integrals in equation 2.29 is discussed below. The boundary-collocation method is used, and the force is assumed to be constant over each boundary element. A procedure for using higher order approximations for the force is described by Hsu and Ganatos [34].

First we write equation 2.29 as

$$\int_{(D)} q_{\alpha\beta}(\hat{\mathbf{x}}) \mathfrak{F}_{\beta} \sigma dl = -8\pi\mu u_{\alpha}^v(\mathbf{x}_0) + \int_{(D_b)} (q_{\alpha\sigma}(\hat{\mathbf{x}}) - q_{\alpha\phi}(\hat{\mathbf{x}})) \kappa\mu \sigma dl \quad (2.32)$$

where $q_{\alpha\beta} = Q_{\alpha\beta}$ for the xx , $x\sigma$, σx , and $\sigma\sigma$ terms; $q_{\alpha\beta} = -Q'_{\alpha\beta}$ for the $x\phi$ and $\sigma\phi$ terms; $q_{\alpha\beta} = Q'_{\alpha\beta}$ for the ϕx and $\phi\sigma$ terms; and curve (D) represents curve $(D_w + D_p)$. As mentioned in the previous section, the procedure for calculating $Q_{\alpha\beta}$ and $Q'_{\alpha\beta}$ is given in Appendix A. Note that $\mathbf{x}_0$ is on the protrusion or the wall so that $-u_{\alpha}^v = u_{\alpha}^{\infty}$.

Next, the curves (D) and (D_b) are divided into N and M elements, respectively, as illustrated in Figure 2.4. Over a given element on curve (D) (*i.e.*, between a given l_i and l_{i+1} on curve (D) in Figure 2.4), the force can be written as

$$\mathfrak{F}_{\beta}(\mathbf{x}) = \mathfrak{F}_{\beta i} + f_{\beta}(\mathbf{x}) \quad (2.33)$$

where $\mathfrak{F}_{\beta}$ and f_{β} are functions of $\mathbf{x}$ and $\mathfrak{F}_{\beta i}$ is a constant over element i . $\mathfrak{F}_{\beta}$ represents the exact value for the unknown function, $\mathfrak{F}_{\beta i}$ represents an approximation to the unknown function over element i , and f_{β} is the difference between the two.

Substituting equation 2.33 into 2.32 gives

$$\begin{aligned} \sum_{i=1}^N \mathfrak{F}_{\beta i} \int_{l_i}^{l_{i+1}} q_{\alpha\beta}(\hat{\mathbf{x}}) \sigma dl + 8\pi\mu R_{\alpha}(\mathbf{x}_0) = \\ -8\pi\mu u_{\alpha}^v(\mathbf{x}_0) + \sum_{m=N+2}^{M+N+2} \kappa\mu \int_{l_m}^{l_{m+1}} (q_{\alpha\sigma}(\hat{\mathbf{x}}) - q_{\alpha\phi}(\hat{\mathbf{x}})) \sigma dl \end{aligned} \quad (2.34)$$

Figure 2.4: Schematic diagram of a mesh established on the appropriate boundaries. Nodes n_j are centered in the elements of curve (D).

where

$$R_\alpha(\mathbf{x}_0) = \frac{1}{8\pi\mu} \int_{(D)} q_{\alpha\beta}(\hat{\mathbf{x}}) f_\beta(\hat{\mathbf{x}}) \sigma \, dl. \quad (2.35)$$

The quantity R_α is called the residue and has the units of velocity. The residue is assumed to be zero when the integrals are evaluated with the pole $\mathbf{x}_0$ placed at any one of N collocation points on the boundary. The collocation points or nodes are placed at the center of each element on curve (D) . The nodes are designated by the symbol n_j in Figure 2.4.

Once the $\mathfrak{F}_{\beta i}$ have been determined, the local residue can be calculated to show that it is negligible by placing the pole at some position on the boundary. The x and σ components of the residue are shown in Figure 2.5 for element number 60, which happens to be on the wall, and for $\phi = 0$ (hemispherical protrusion geometry; 40 elements on the hemisphere; 60 elements on the wall; constant element spacing on both the protrusion and wall). The ϕ component of the residue is zero for $\phi = 0$. The residue was made dimensionless by κR , which is the shear rate at the wall times the radius of the hemisphere. The residue is plotted against the dimensionless position of the pole. At -1 and 1, the pole is at the element edges, and at 0 the pole is at one of the collocation points. As prescribed, the residue is zero at the collocation point and small away from the collocation point.

The boundary-collocation method, with the force approximated as a constant, results in a set of $3N$ equations and $3N$ unknowns. The matrix of equation can be written as

$$\begin{aligned} \sum_{i=1}^N \mathfrak{F}_{\beta i} K_{ij}^{\alpha\beta} &= U_j^\alpha + S_j^\alpha \\ K_{ij}^{\alpha\beta} &= \int_{l_i}^{l_{i+1}} q_{\alpha\beta}(\hat{\mathbf{x}}) \sigma \, dl \\ U_j^\alpha &= -8\pi\mu u_\alpha^v(\mathbf{x}_j) \\ S_j^\alpha &= \sum_{m=N+2}^{M+N+2} \kappa\mu \int_{l_m}^{l_{m+1}} (q_{\alpha\sigma}(\hat{\mathbf{x}}) - q_{\alpha\phi}(\hat{\mathbf{x}})) \sigma \, dl \end{aligned} \quad (2.36)$$

where $\mathbf{x}_0 = \mathbf{x}_j$ and $\hat{\mathbf{x}} = \mathbf{x} - \mathbf{x}_j$. $K_{ij}^{\alpha\beta}$ occupies the i th row and the j th column of the matrix on the left side of equation 2.36, and the quantity $(U_j^\alpha + S_j^\alpha)$ occupies the j th column

Figure 2.5: A spot-check calculation of the x and σ components of the residue along an element for a hemispherical protrusion. The residue is normalized by the product of the shear rate and the hemisphere radius. At a dimensionless position of -1 and 1 the pole is at the element edges, and at 0 the pole is at a collocation point.

position on the right side of equation 2.36.

Line segments or circular arc segments represent the curves (D) and (D_b) in our mesh. For a line segment defined by the points (x_i, σ_i) and (x_{i+1}, σ_{i+1}) , dl is given by

$$\begin{aligned} \text{for } x_{i+1} \neq x_i \quad dl &= \sqrt{(a^2 + 1)} |dx| = \alpha \sqrt{(a^2 + 1)} dx \\ \alpha &= \frac{x_{i+1} - x_i}{|x_{i+1} - x_i|} \quad a = \frac{\sigma_{i+1} - \sigma_i}{x_{i+1} - x_i} \\ \text{for } x_{i+1} = x_i \quad dl &= |d\sigma| = \alpha d\sigma \\ \alpha &= \frac{\sigma_{i+1} - \sigma_i}{|\sigma_{i+1} - \sigma_i|} \end{aligned} \quad (2.37)$$

and for a circular arc defined by a radius, R , a center point, $\mathbf{x}_c$, and two angles, ψ_i and ψ_{i+1} , dl is given by

$$\begin{aligned} dl &= R |d\psi| = \alpha R d\psi \\ \alpha &= \frac{\psi_{i+1} - \psi_i}{|\psi_{i+1} - \psi_i|} \end{aligned} \quad (2.38)$$

Before evaluating 2.36, it is convenient to change the limits of integration from l_i to l_{i+1} to -1 to 1. Using $K_{ij}^{\alpha\beta}$ as an example

$$\begin{aligned} K_{ij}^{\alpha\beta} &= \int_{-1}^1 q_{\alpha\beta}(\hat{\mathbf{x}}) \sigma \frac{dl}{d\xi} d\xi \\ l &= \frac{l_{i+1} - l_i}{2} \xi + \frac{l_{i+1} + l_i}{2} \\ \frac{dl}{d\xi} &= \frac{l_{i+1} - l_i}{2} \end{aligned} \quad (2.39)$$

where $(l_{i+1} - l_i)/2$ can be found for a line by integrating equation 2.37

$$\begin{aligned} \text{for } x_{i+1} \neq x_i \quad \frac{l_{i+1} - l_i}{2} &= \alpha \sqrt{(a^2 + 1)} \left(\frac{x_{i+1} - x_i}{2} \right) \\ \text{for } x_{i+1} = x_i \quad \frac{l_{i+1} - l_i}{2} &= \alpha \left(\frac{\sigma_{i+1} - \sigma_i}{2} \right) \end{aligned} \quad (2.40)$$

and for an arc by integrating equation 2.38

$$\frac{l_{i+1} - l_i}{2} = \alpha R \left(\frac{\psi_{i+1} - \psi_i}{2} \right) \quad (2.41)$$

Six-point Gaussian integration formulas were used to evaluate the integrals $K_{ij}^{\alpha\beta}$ and S_j^α after they were changed to the form given by 2.39. Gaussian integration formulas are reported by Abramowitz and Stegun [35].

When $i = j$, care must be taken when evaluating the integrals $K_{ij}^{\alpha\beta}$ since the pole $\mathbf{x}_0$ is in the center of the element of integration. As $\mathbf{x}$ approaches $\mathbf{x}_0$ the functions Q_{xx} , $Q_{\sigma\sigma}$, and $Q_{\phi\phi}$ increase towards infinity as fast as the functions $-2\ln(|\hat{\mathbf{x}}|)$, $-2\ln(|\hat{\mathbf{x}}|)$, and $-4\ln(|\hat{\mathbf{x}}|)$ increase toward infinity. This is true whether the free-space Green's function or the wall Green's function is used to calculate the $Q_{\beta\beta}$ values. The reason for the appearance of the logarithmic singularities is discussed in Appendix A.6. The problem does not occur for the integrals S_j^α since the poles are never placed on curve D_b .

To deal with the singularities, the quantity $\mathfrak{F}_{\beta i} K_{jj}^{\beta\beta}$ is written as

$$\begin{aligned} \mathfrak{F}_{\beta i} K_{jj}^{\beta\beta} &= \mathfrak{F}_{\beta i} \left\{ \int_{-1}^1 [q_{\beta\beta} \sigma + (\text{factor}) \ln |l - l_0| - (\text{factor}) \ln |l - l_0|] \frac{dl}{d\xi} d\xi \right\} \\ &= \mathfrak{F}_{\beta i} \left\{ \int_{-1}^1 [q_{\beta\beta} \sigma + (\text{factor}) \ln |l - l_0|] \frac{dl}{d\xi} d\xi \right. \\ &\quad \left. - (\text{factor}) \int_{l_i}^{l_{i+1}} \ln |l - l_0| dl \right\} \quad (2.42) \end{aligned}$$

where factor = 2, 2, or 4 for $\beta\beta = xx$, $\sigma\sigma$, or $\phi\phi$. The right-most integral in 2.42 is evaluated analytically. It can be written as

$$(\text{factor}) \int_{l_i}^{l_{i+1}} \ln |l - l_0| dl = 2 (\text{factor}) |l_i - l_0| (1 - \ln |l_i - l_0|) \quad (2.43)$$

because $|l_{j+1} - l_0| = |l_j - l_0|$. Note that $|l_j - l_0|$ can be found for a line or an arc by integrating equations 2.37 and 2.38.

The integrand $[q_{\beta\beta} \sigma + (\text{factor}) \ln |l - l_0|]$ in equation 2.42 changes smoothly over the singularity. Hence, equation 2.42 can be evaluated numerically with accuracy. Although the integrand as a whole is finite at the pole, $q_{\beta\beta}$ is infinite at the pole. If a Gaussian integration formula were used with an odd number of points, then the integrand would need to be evaluated in the limit of $\mathbf{x} \rightarrow \mathbf{x}_0$ for the integration point on the pole.

The above procedure results in a full matrix, as opposed to the diagonal matrices obtained by finite-element techniques. The matrix was solved using the subroutines LUDCMP and LUBKSB from *Numerical Recipes* [36]. LUDCMP decomposes a row-wise permutation of the matrix of equations into a lower and upper triangular matrix. LUBKSB

returns the solution using the lower and upper triangular matrices as input. A typical matrix size was 300×300 for the free-space Green's function and 200×200 for the wall Green's function. The calculations were performed on a DEC Station 5000 from Digital Equipment Corporation. The time to fill and solve a 300×300 matrix is approximately 40 s + 60 s = 100 s for the free-space Green's function and 80 s + 60 s = 140 s for the wall Green's function.

Once the unknown coefficients, $\mathfrak{F}_{\beta i}$, have been calculated, local velocities can be determined. The equation for the velocity at any position $\mathbf{x}_0$ inside the domain is obtained by rearranging equation 2.34 to give

$$u_{\alpha}(\mathbf{x}_0) = -\frac{1}{8\pi\mu} \sum_{i=1}^N \mathfrak{F}_{\beta i} \int_{l_i}^{l_{i+1}} q_{\alpha\beta}(\hat{\mathbf{x}}) \sigma dl + u_{\alpha}^{\infty}(\mathbf{x}_0) + \frac{1}{8\pi\mu} \sum_{m=N+2}^{M+N+2} \kappa\mu \int_{l_m}^{l_{m+1}} (q_{\alpha\sigma}(\hat{\mathbf{x}}) - q_{\alpha\phi}(\hat{\mathbf{x}})) \sigma dl \quad (2.44)$$

where the residual R_{α} has been assumed to be negligible. The velocities were always calculated using the wall Green's function since it is more accurate, especially for trajectories that come very close to the wall.

2.6 Generation of flow trajectories

Flow trajectories were calculated by applying the modified Euler method to the ordinary differential equation

$$dt = \frac{dx}{u_x} = \frac{d\sigma}{u_{\sigma}} = \sigma \frac{d\phi}{u_{\phi}}. \quad (2.45)$$

First, a step size t and starting position (x_1, σ_1, ϕ_1) are selected. The velocities u_{x1} , $u_{\sigma1}$, and $u_{\phi1}$ are then determined at the starting position using equation 2.44. A first guess can be found for position 2 by integrating equation 2.45 to obtain

$$\begin{aligned} x_2 &= x_1 + u_{x1} t \\ \sigma_2 &= \sigma_1 + u_{\sigma1} t \\ \phi_2 &= \phi_1 + \left(\frac{2u_{\phi1}}{\sigma_1 + \sigma_2} \right) t \end{aligned} \quad (2.46)$$

where the velocities were assumed to be constant over the time step and σ was approximated by $(\sigma_1 + \sigma_2)/2$.

The velocities u_{x2} , $u_{\sigma 2}$, and $u_{\phi 2}$ are then calculated at position 2. An improved guess for position 2 then can be calculated using equation 2.46 with the average of the velocities at positions 1 and 2 in place of the initial value for the velocity. This procedure is repeated until convergence is achieved. The subsequent points along the flow trajectory are calculated in the same manner.

2.7 Generation of skin-friction lines

Skin-friction lines are the same as limiting streamlines, flow paths immediately adjacent to the boundaries. A common experimental method for visualizing skin-friction lines is the oil-flow method (see [37], Chapter X, Section 15). Also, skin-friction lines near the surface of a rotating disk electrode can be visualized in the electrodeposition pattern of zinc [21]. The boundary-integral technique is ideally suited for the generation of skin-friction lines because one directly solves for the surface force, which is directly proportional to the velocity close to the boundary.

The differential equation for the generation of skin-friction lines is

$$dt = \frac{dS}{u_{sl}} = \sigma \frac{d\phi}{u_{\phi l}}. \quad (2.47)$$

S is the parametric distance along the trace of the protrusion and the wall at some angle ϕ (see Figure 2.6), and dS is a differential step along this curve. S is zero at the top of the protrusion. The velocity component u_{sl} points in the direction of increasing S . The subscript l on u_{sl} and $u_{\phi l}$ indicates that these quantities are proportional to velocities very close to the surface.

To determine u_{sl} and $u_{\phi l}$, the shear stress at the wall, τ_w , is required. The wall

Figure 2.6: The distance, S , is defined as the parametric distance along the trace of the protrusion and the wall at some angle ϕ . S is zero at the top, center of the protrusion.

shear is given by

$$\begin{aligned}\vec{\tau}_w &= [(f_x \vec{i}_x + f_\sigma \vec{i}_\sigma) \cdot \vec{t}] \vec{t} + f_\phi \vec{i}_\phi \\ &= \mu \frac{du_{sl}}{dn} \vec{t} + \mu \frac{du_{\phi l}}{dn} \vec{i}_\phi\end{aligned}\quad (2.48)$$

where $\vec{i}_x$, $\vec{i}_\sigma$, $\vec{i}_\phi$ are unit vectors in the x , σ , and ϕ directions; $\vec{t}$ is a tangent vector that points in the direction of increasing S ; and dn is the differential distance normal to the surface. Replacing the differential quantities du_{sl} , $du_{\phi l}$, and dn in equation 2.48 with the discrete quantities u_{sl} , $u_{\phi l}$, and n and rearranging, one obtains

$$\begin{aligned}u_{sl} &= \frac{n}{\mu} (f_x \vec{i}_x + f_\sigma \vec{i}_\sigma) \cdot \vec{t} \\ u_{\phi l} &= \frac{n}{\mu} f_\phi.\end{aligned}\quad (2.49)$$

for the velocities u_{sl} and $u_{\phi l}$.² Substituting equation 2.49 into equation 2.47 gives

$$dt = \frac{\mu}{n} \frac{dS}{(f_x \vec{i}_x + f_\sigma \vec{i}_\sigma) \cdot \vec{t}} = \sigma \frac{\mu}{n} \frac{d\phi}{f_\phi}. \quad (2.50)$$

Integrating equation 2.50 over a time step t and rearranging the resulting equation yields

$$\begin{aligned} S_2 &= S_1 + (f_{x1} \vec{i}_x + f_{\sigma 1} \vec{i}_\sigma) \cdot \vec{t} \left(\frac{nt}{\mu} \right) \\ \phi_2 &= \phi_1 + \left(\frac{2f_{\phi 1}}{\sigma_1 + \sigma_2} \right) \left(\frac{nt}{\mu} \right) \end{aligned} \quad (2.51)$$

where the quantities $(f_{x1} \vec{i}_x + f_{\sigma 1} \vec{i}_\sigma) \cdot \vec{t}$ and $f_{\phi 1}$ were held constant at their initial values as indicated by the subscript 1 and the average quantity $(\sigma_1 + \sigma_2)/2$ was used to approximate σ .

The initial position of the streak line is (S_1, ϕ_1) . To calculate the second position on the surface, equation 2.51 and an equation for σ_1 and σ_2 are needed. There is a one-to-one correspondence between σ and S , but since the relation depends upon the protrusion geometry, a general equation is not given. With the additional relations for σ_1 and σ_2 , equation 2.51 has the same form as equation 2.46. Instead of choosing a time step t , however, one chooses a value for the quantity $(nt)/(\mu)$. Otherwise, the procedure is the same as the procedure for generating flow trajectories.

2.8 Shear-stress distributions over axisymmetric protrusions

In this section, we present the dimensionless shear-stress distribution, τ_w/τ_w^∞ , for both spherical-type protrusions and cylindrical-type protrusions. Figure 2.7 shows the salient features of these protrusion types. The spherical-type protrusions are sections of a sphere with radius a , semi-angle α , and curvature R . The cylindrical-type protrusions are characterized by a height-to-radius ratio, h/a . The cylinder in Figure 2.7 is drawn with rounded corners with a radius of curvature, r_c , but, unless explicitly stated, the cylindrical protrusions should be assumed to have sharp corners.

²One can derive equation 2.49 independently of equation 2.48. For example, on the side of a cylindrical protrusion, $f_\phi = \mu \sigma \frac{d}{d\sigma} \left(\frac{u_\phi}{\sigma} \right)$. Rearranging and integrating from the surface of the cylinder (σ_0) to a finite distance from the cylinder ($\sigma_0 + \sigma$) results in $\frac{d\phi}{dt} = \frac{f_\phi}{\mu} \ln(1 + \frac{\sigma}{\sigma_0})$. Expanding the logarithmic term in a Taylor series about 1 and rearranging gives $\sigma \frac{d\phi}{dt} = \frac{\sigma}{\mu} f_\phi$, which is the same as equation 2.49.

Figure 2.7: Definition of length scales.

The shear stress given by equation 2.48 can be expanded using equation 2.16 to

$$\vec{\tau}_w = [(\mathfrak{F}_x \cos(\phi) \vec{i}_x + \mathfrak{F}_\sigma \cos(\phi) \vec{i}_\sigma) \cdot \vec{t}] \vec{t} - \mathfrak{F}_\phi \sin(\phi) \vec{i}_\phi. \quad (2.52)$$

For $\phi=0^\circ$, equation 2.52 reduces to

$$\vec{\tau}_w = [(\mathfrak{F}_x \vec{i}_x + \mathfrak{F}_\sigma \vec{i}_\sigma) \cdot \vec{t}] \vec{t} \quad \text{for } \phi=0^\circ, \quad (2.53)$$

and for $\phi=-90^\circ$, it reduces to

$$\vec{\tau}_w = \mathfrak{F}_\phi \vec{i}_\phi \quad \text{for } \phi=-90^\circ. \quad (2.54)$$

If $\phi = 180^\circ$ and $\phi = 90^\circ$ were used to reduce equation 2.52 instead, then the right side of equations 2.53 and 2.54 would be multiplied by -1. This is because the $\vec{i}_x$ and $\vec{i}_\sigma$ components of the shear stress are antisymmetric about the xz-plane and the $\vec{i}_\phi$ component is antisymmetric about the xy-plane.

In each of the figures in this section, the dimensionless shear-stress is plotted against dimensionless arc length S/a for $\phi = 0^\circ$ and $\phi = -90^\circ$. These angles were chosen because they correspond to positive values of the shear stress near the common point at the top of the protrusion, producing the most visually appealing plots. The angle $\phi = -90^\circ$ will be referred to as the transverse direction, and the angle $\phi = 0^\circ$ will be referred to as the downstream direction or the flow direction.

For the spherical-type protrusions, $\vec{t} = -\sin(\theta) \vec{i}_x + \cos(\theta) \vec{i}_\sigma$ on the protrusion, and $\vec{t} = \vec{i}_\sigma$ on the wall. The angle θ is shown in Figure 2.3. Hence, equation 2.53 becomes

$$\begin{aligned} \vec{\tau}_w &= [-\mathfrak{F}_x \sin(\theta) + \mathfrak{F}_\sigma \cos(\theta)] \vec{t} \quad \text{for } \phi = 0^\circ \text{ on the sphere} \\ &= \mathfrak{F}_\sigma \vec{i}_\sigma \quad \text{for } \phi = 0^\circ \text{ on the wall} \end{aligned} \quad (2.55)$$

For the cylindrical-type protrusions, $\vec{t} = \vec{i}_\sigma$ on top of the protrusions and on the wall, and $\vec{t} = -\vec{i}_x$ on the side of the cylinder. Equation 2.53 becomes

$$\begin{aligned} \vec{\tau}_w &= -\mathfrak{F}_x \vec{i}_x \quad \text{for } \phi = 0^\circ, \text{ cylinder side} \\ &= \mathfrak{F}_\sigma \vec{i}_\sigma \quad \text{for } \phi = 0^\circ, \text{ cylinder top and wall} \end{aligned} \quad (2.56)$$

For $\phi = -90^\circ$, $\vec{\tau}_w = \mathfrak{F}_\phi \vec{i}_\phi$ for both protrusion geometries everywhere on the surface. The functions corresponding to $\vec{\tau}_w$ are marked directly on the shear-stress distribution curves in Figures 2.8 to 2.12. The symbols F are used instead of $\mathfrak{F}$ because of the limitations of our plotting program.

The shear-stress distributions can be split into a protrusion region and a wall region. For each plot, the stress distributions for $\phi = 0^\circ$ and -90° both approach zero at a single value of S/a . This value of S/a marks the boundary between the protrusion and the wall.

On the wall, downstream of a protrusion, negative shear stresses indicate that fluid is flowing opposite to the direction of bulk fluid flow. The corresponding positive shear stresses on the wall, upstream of a protrusion (the $\vec{i}_x$ and $\vec{i}_r$ components of the shear stress are antisymmetric about the xz -plane) also indicate that fluid is flowing opposite to the direction of bulk fluid flow. On the side of a cylindrical protrusion—both upstream and downstream—negative shear stresses indicate that fluid is flowing vertically toward the wall, and positive shear stresses indicate that fluid is flowing vertically away from the wall. This means that fluid which flows toward the wall on one side of a protrusion flows away from the wall at the corresponding position on the opposite side of the protrusion because the $\vec{i}_x$ component of the shear stress is antisymmetric about the xz -plane. In the following discussion, “flow reversal regions” correspond to regions where the fluid flows opposite to the direction of bulk fluid flow. By this definition, flow reversal regions do not occur along the sides of cylinders.

First, the stress distributions for spherical-type protrusions with $\alpha=34^\circ$ and 90° are examined in Figures 2.8 and 2.9. A sketch of the appropriate protrusion is drawn on each graph. To see a greater range of semi-angles, the reader is referred to Pozrikidis [32]. For both semi-angles, the shear stress at $\phi=-90^\circ$ is greater than the shear stress at $\phi=0^\circ$. The maximum dimensionless shear stress occurs at the top of the protrusions and is just over 2.0 for $\alpha = 34^\circ$ and just over 4 for $\alpha = 90^\circ$.

As mentioned above, the shear stress near the intersection between the protrusion

Figure 2.8: The dimensionless shear-stress distribution, τ_w / τ_w^∞ , for a protrusion that is a section of a sphere with radius a and semi-angle $\alpha = 34^\circ$, as defined in Figure 2.7. The solid line (labeled $\phi = 0^\circ$) is the stress distribution along the flow direction. The dotted line (labeled $\phi = -90^\circ$) is the stress distribution along the transverse direction. The abscissa is the dimensionless arc length defined in Figure 2.6.

Figure 2.9: The dimensionless shear-stress distribution, τ_w / τ_w^∞ , for a hemispherical protrusion ($\alpha = 90^\circ$). The radius is a . The solid line (labeled $\phi = 0^\circ$) is the stress distribution along the flow direction. The dotted line (labeled $\phi = -90^\circ$) is the stress distribution along the transverse direction. The abscissa is the dimensionless arc length defined in Figure 2.6.

and the wall approaches zero for both semi-angles along the flow and transverse directions. However, the shear stress for $\alpha = 34^\circ$ never passes below zero, but the shear stress for $\alpha = 90^\circ$ passes through zero on the protrusion and on the wall. The flow parallel to the surface changes direction at each of these points. Points of zero shear stress will be referred to as stagnation points or as singular points. The term "singular point" will be used primarily when flow trajectories are discussed. Depending on the protrusion geometry, a total of 2 to 4 stagnation points could be resolved. In two-dimensional flows, when two planes meet at an angle less than 124° ($34^\circ + 90^\circ$), an infinite sequence of stagnation points are encountered as the corner is approached due to an infinite sequence of counter-rotating vortices. These vortices are called Moffatt eddies after Moffatt's classical paper on the subject [38]. For axisymmetric protrusions, the largest semi-angle for which no flow reversal is observed in the xy-plane is approximately 34° . Since the critical angle is the same, this suggests that an infinite sequence of eddies also exists for axisymmetric protrusions in the xy-plane when $\alpha > 34^\circ$, but this is not demonstrated explicitly.

We found a stagnation point at $\theta = 73.2^\circ$ on the hemisphere and at $y/a = 1.22$ on the wall, which are the same values calculated by Price [31]. At $\theta = 73.2^\circ$ the flow separates from the hemisphere, but it does not re-attach at $y/a = 1.22$ on the wall as one might be led to believe by Price's discussion. As we shall see later, there is a vortex near the stagnation point on the wall, and the flow trajectory that detaches from the protrusion never re-attaches to the wall.

We now turn our attention to shear-stress distributions for cylindrical protrusions. The distributions in Figures 2.10 to 2.12 are for cylinders with aspect ratios of $h/a=0.5$, 2, and 8. A drawing of the appropriate cylindrical protrusion is included with each figure.

The most dramatic difference in the stress distributions between the spherical- and the cylindrical-type protrusions is the rapid increase in the shear stress to infinity near the sharp corners at the top of the cylinders. In general, the shear-stress distributions appear to change more abruptly over the cylinders than over the spherical-type protrusions. Also, distinct negative values for the shear stress are observed on the side of the cylinders in

Figure 2.10: The dimensionless shear-stress distribution, τ_w / τ_w^∞ , for a cylindrical protrusion with a height-to-radius ratio of $h/a = 0.5$. The solid line (labeled $\phi = 0^\circ$) is the stress distribution along the flow direction. The dotted line (labeled $\phi = -90^\circ$) is the stress distribution along the transverse direction. The abscissa is the dimensionless arc length defined in Figure 2.6.

Figure 2.11: The dimensionless shear-stress distribution, τ_w / τ_w^∞ , for a cylindrical protrusion with a height-to-radius ratio of $h/a = 2$. The solid line (labeled $\phi = 0^\circ$) is the stress distribution along the flow direction. The dotted line (labeled $\phi = -90^\circ$) is the stress distribution along the transverse direction. The abscissa is the dimensionless arc length defined in Figure 2.6.

Figure 2.12: The dimensionless shear-stress distribution, τ_w / τ_w^∞ , for a cylindrical protrusion with a height-to-radius ratio of $h/a = 8$. The solid line (labeled $\phi = 0^\circ$) is the stress distribution along the flow direction. The dotted line (labeled $\phi = -90^\circ$) is the stress distribution along the transverse direction. The abscissa is the dimensionless arc length defined in Figure 2.6.

comparison to the negative values on the hemisphere. There are also similarities in the stress distributions. For both geometries, the shear stress on the wall recovers to unity (its undisturbed value) much faster along the transverse direction than along the flow direction. Also, the shear stress at any given value of S/a is greater at $\phi=-90^\circ$ than at $\phi=0^\circ$, although the difference on top of the cylinders is very small. This means that, to a first approximation, the shear stress depends on radial distance but not on ϕ on top of the cylinders.

The shear stress at $S = 0$ (the point at the top of the cylinder along the x-axis) increases more slowly than the aspect ratio. Between $h/a=0.5$ and 8, the aspect ratio increases by a factor of 16, while the shear stress at the top center of the cylinders increases from, approximately, $\tau_w/\tau_w^\infty=1.5$ to 6, a factor of only 4. However, since h/a starts at 0 and τ_w/τ_w^∞ starts at 1, 1 should be subtracted from τ_w/τ_w^∞ to make the comparison more legitimate. Still, this adjusted ratio, $5/0.5=10$, is lower than the ratio of the h/a values. On the wall surrounding the cylinders, the magnitude of the flow reversal region decreases significantly with increasing aspect ratio. At $h/a = 0.5$ there is a distinct flow reversal region, at $h/a = 2$ the flow reversal region is noticeable but very weak, and at $h/a = 8$ it is virtually nonexistent.

The locations of the resolvable stagnation points for cylindrical protrusions of various aspect ratios are shown in Table 2.1. The aspect ratio range is from $h/a = 0.1$ to $h/a = 8$. On the side of the protrusions, the distance from the wall (x/h) of each of the stagnation points is given. On the wall, the downstream locations (y/a) of the stagnation points are given. There are no stagnation points along the transverse direction. As the aspect ratio of the protrusion increases, the stagnation point on the side of the protrusion moves farther from the wall, but it is within 15% of the top of the protrusion for the entire aspect-ratio range. The outer-most stagnation point on the wall was resolvable for $h/a=0.1$ to 2.4, and it was located the farthest from the protrusion at $h/a=2$. The second outer-most stagnation point was resolvable for $h/a=2$ and 2.4; it could not be resolved at lower aspect ratios when this stagnation point is very close to the protrusion. As the aspect ratio increases, the second outer-most stagnation point begins moving away from the

Table 2.1: The location of some stagnation points ($\tau_w/\tau_w^\infty = 0$) for cylindrical protrusions of various h/a . The cylinders have sharp corners. On the side of each cylinder, the distance from the wall (x/h) of the top-most stagnation point is given. On the wall, the downstream location (y/a) of the outer-most and 2nd outer-most stagnation points are given, provided that they could be resolved.

h/a	Stagnation points, $\tau_w/\tau_w^\infty = 0$		
	on the side of the protrusion x/h	on the wall	
		the 2nd outer-most stagnation point y/a	the outer-most stagnation point y/a
0.1	0.864	*	1.08
0.5	0.889	*	1.33
1	0.905	<1.1	1.52
2	0.922	1.15	1.60
2.4	0.925	1.24	1.49
2.6	0.926	*	*
4	0.933	*	*
8	0.941	*	*

* could not be resolved

protrusion and approaches the outer-most stagnation point. These two stagnation points come together and disappear somewhere between $h/a=2.4$ and $h/a=2.6$, and no stagnation points are resolvable on the wall at higher aspect ratios.

Only the shear-stress distributions on the top of cylinders are shown in Figure 2.13 for $h/a=0.1$ to 8. The stress is plotted against dimensionless radial distance, σ/a . The shear-stress distributions are somewhat similar for the different aspect ratios, and the shear stress at a given value of σ/a is only slightly greater along the transverse direction than along the flow direction. The shear stress monotonically increases with aspect ratio. Only the shear-stress distributions on the side of cylinders are plotted in Figure 2.14 for the same aspect ratio range. The stress is plotted against the dimensionless distance from the top of the protrusion ($1 - x/h$). The ordinate has the same scale as in Figure 2.13. The stress distributions change more rapidly with aspect ratio for $\phi = -90^\circ$ than for $\phi = 0^\circ$. For $\phi = -90^\circ$, the shear stress increased with aspect ratio, and for $\phi = 0^\circ$, the magnitude of the negative shear stress increases. The shear stress for $\phi = 0^\circ$ passes through zero very

Figure 2.13: The dimensionless shear-stress distribution, τ_w / τ_w^∞ , on the top of cylindrical protrusions for h/a equal to 0.1, 0.5, 2, 4, and 8. The solid line is the stress distribution along the radial direction at $\phi = 0^\circ$ (downstream direction). The dotted line is the stress distribution along the radial direction at $\phi = -90^\circ$.

close to the top of the protrusion, and this point appears at larger x/h as the aspect ratio increases. This is more clearly evident in the inset graph in Figure 2.14.

2.9 Stress contours for cylindrical protrusions

Figure 2.15 shows contours of the magnitude of the dimensionless shear stress ($|\tau_w|/\tau_w^\infty$, see equation A.33 in Appendix A.3) from a top view for cylindrical protrusions with $h/a = 0.5, 2$, and 8 . Figure 2.16 shows a close up of the same contours. The maximum stress contour is $|\tau_w|/\tau_w^\infty = 0.8$ in each plot. The magnitude of the shear stress is plotted because it is continuous whereas the vector quantity is not. The abscissa on each of the plots is the dimensionless distance in the flow direction, y/a , and the ordinate is the dimensionless distance in the transverse direction, z/a . The dotted lines are the stress contours, and the dashed lines mark the boundary of the protrusions. Within the boundaries of the solid lines, the y -component of the shear stress is negative. Hence the solid lines can be thought of as the boundaries of the flow-reversal region on the wall. The asterisks mark the location of stagnation points, which lie on the boundary of the flow-reversal regions. The second outer-most stagnation points are marked for $h/a = 0.5$ in the stress contours, but they were not included in Table 2.1. This was because the position of this stagnation point could not be resolved to 3-digit accuracy.

It can be readily seen from Figure 2.15 that the radial extent of the disturbance significantly increases with aspect ratio in the flow direction, but the extent of the disturbance in the transverse direction increases only gradually. Hence, as the aspect ratio increases, the stress contours assume a characteristic dumbbell shape. The extent of the stress disturbance is quantified for aspect ratios between 0.1 and 8 in Table 2.2. The downstream/upstream positions ($|y|/a$) and the transverse positions ($|z|/a$) at which the shear stress recovers to the values $\tau_w/\tau_w^\infty = 0.8, 0.9, 0.95$, and 0.98 are given in the table. For $h/a = 8$, it takes over 31 radii for the shear stress to recover to 98% of its value at infinity along the flow direction, but only 4.76 radii to recover to the same value along the transverse

Figure 2.14: The dimensionless shear-stress distribution, τ_w / τ_w^∞ , on the side of cylindrical protrusions for h/a equal to 0.1, 0.5, 2, 4, and 8. The solid line is the stress distribution at $\phi = 0^\circ$. The dashed line is the stress distribution at $\phi = -90^\circ$. The abscissa, $1 - (x/h)$, is the dimensionless distance from the top of the protrusion towards the wall.

Figure 2.15: Contours of the magnitude of the dimensionless wall shear stress, $|\tau_w|/\tau_w^\infty$, for cylindrical protrusions of different heights as viewed by an observer looking down on the protrusions ($h/a = 0.5, 2$, and 8). The dotted lines are the stress contours; the dashed lines mark the radial boundary of the protrusions; the y-component of the shear stress is negative within the boundaries of the solid lines; and the asterisks mark the location of stagnation points.

Figure 2.16: A close up of the contours in Figure 2.15.

Table 2.2: The extent of the wall shear stress disturbance for cylindrical protrusions of various aspect ratios, h/a , and for various values of $|\tau_w|/\tau_w^\infty$.

h/a	$ y /a$ values along the flow direction				$ z /a$ values to either side of the protrusion			
	$ \tau_w /\tau_w^\infty$				$ \tau_w /\tau_w^\infty$			
	0.8	0.9	0.95	0.98	0.8	0.9	0.95	0.98
0.1	1.38	1.58	1.87	2.40	1.14	1.21	1.30	1.46
0.5	2.38	2.95	3.68	4.95	1.38	1.57	1.77	2.10
0.65	2.68	3.37	4.23	5.71	1.44	1.65	1.89	2.25
1	3.33	4.25	5.39	7.34	1.53	1.80	2.10	2.54
2	4.94	6.46	8.30	11.4	1.69	2.07	2.50	3.13
4	7.70	10.3	13.4	18.6	1.82	2.36	2.97	3.88
8	12.5	17.1	22.6	31.7	1.90	2.57	3.41	4.76

direction. For $h/a = 0.1$, on the other hand, the corresponding values are only 2.4 radii and 1.46 radii. To attain 3-digit accuracy for these values, the positions were calculated using the wall Green's function.

The size of the recirculation regions is shown in Figure 2.16. The region for $h/a=0.5$ extends farther in the transverse direction than for $h/a=2$, but the region for $h/a=2$ extends farther downstream. The dimensionless shear stress is higher in the recirculation region for the lower aspect ratio. Specifically, the stress contours for $|\tau_w|/\tau_w^\infty=0.1$ and 0.2 intersect the flow-reversal boundary for $h/a=0.5$, but the entire boundary lies within the 0.1 stress contour for $h/a=2$. At $h/a=8$, the recirculation region has completely disappeared. Hence, with the aid of Table 2.1 we come to the following conclusions. As the aspect ratio of the protrusion increases, the recirculation region becomes narrower in the transverse direction, moves away from the protrusion, becomes weaker in strength, and extends farther in the flow direction. Then, somewhere between h/a of 2.4 and 2.6, the recirculation region becomes smaller in both directions and completely disappears.

In Figure 2.17, stress contours on the side of cylindrical protrusions are plotted for $h/a=0.5$, 2, and 8. The cylinder has been unscrolled and laid flat, and only the downstream end is viewed, centered around $\phi=0$. The vertical axis is the dimensionless distance from

the wall (x/h), and the abscissa is the angle in degrees around the side of the protrusion. The dashed line marks the top border of the protrusion, and the physical sizes of the graphs are the same.

In general, the fluid experiences diminishing shear stresses as it travels around the protrusion from $\phi = 90^\circ$ to 0° . If one arbitrarily takes the stress contour equal to 1 as the border between the high- and low-shear-stress regions, then the region of low shear stress for $h/a=8$ is concentrated near $\phi = 0^\circ$ and near the wall. As the aspect ratio of the protrusion decreases, the low shear stress region envelopes a larger fraction of the protrusion surface. At $h/a=0.5$, the shear stress is less than 1 on almost the entire side of the protrusion except near the top. Notice that there is a stagnation point at $\phi = 0^\circ$ near the top of each protrusion, and the shear stress increases more rapidly away from this point at the higher aspect ratios. Finally, we note that if the total dimensionless force were proportional to surface roughness, one would expect the stress contours in Figure 2.17 to be identical for all aspect ratios. However, since a larger portion of the protrusion is enveloped by the high-shear-stress region at the higher aspect ratios, the total dimensionless force should increase faster than the roughness, as is the case.

2.10 The total force on cylindrical protrusions with sharp and rounded corners

The total dimensionless force and torque on cylindrical protrusions with sharp and rounded corners is presented in Table 2.3. The calculation procedures are given in Appendix A.8. The total force could be resolved over a greater aspect ratio range than the total torque. The force is normalized by the total force that would be exerted on the base of the protrusion if the protrusion were not present, $\pi\mu\kappa a^2$. The total torque, which is calculated about the origin, is normalized by $\pi\mu\kappa a^3$. The rounded corners have a radius of curvature, r_c , of $0.1a$. Both a and r_c are shown schematically in Figure 2.7. Also, the roughness (the ratio of the surface area of the protrusion divided by the surface area of the

Figure 2.17: Contours of the magnitude of the dimensionless wall shear stress, $|\tau_w|/\tau_w^\infty$, on the side of cylindrical protrusions with height-to-radius ratios, h/a equal to 0.5, 2, and 8. The dotted lines are the stress contours; the dashed lines mark the top boundaries of the protrusions; and the asterisks mark the location of stagnation points.

Table 2.3: The y component of the total force, F_y , and the z component of the total torque, T_z , for cylindrical protrusions of various aspect ratios, h/a . The protrusions have both sharp and rounded corners. The torque is calculated about the origin. The rounded corners have a radius of curvature of $r_c = 0.1a$ (see Figure 2.7). The roughness* of each protrusion is given for comparison.

h/a	$F_y/\pi\mu\kappa a^2$		$T_z/\pi\mu\kappa a^3$		roughness	
	sharp corner	rounded corner	sharp corner	rounded corner	sharp corner	rounded corner
0.01	1.08	—	—	—	1.02	—
0.05	1.31	—	—	—	1.10	—
0.1	1.57	1.46	0.188	0.113	1.20	1.113
0.2	2.08	1.98	0.450	0.357	1.40	1.313
0.3	2.60	2.49	0.786	0.676	1.60	1.513
0.4	3.12	3.01	1.20	1.07	1.80	1.713
0.5	3.65	3.54	1.70	1.55	2.00	1.913
0.6	4.20	4.08	2.28	2.11	2.20	2.113
0.65	4.48	4.36	2.60	2.42	2.30	2.213
0.7	4.76	4.64	2.94	2.76	2.40	2.313
0.8	5.34	5.21	3.70	3.49	2.60	2.513
0.9	5.93	5.80	4.55	4.32	2.80	2.713
1.0	6.54	6.40	5.49	5.25	3.00	2.913
1.5	9.80	9.65	11.8	11.4	4.00	3.913
2.0	13.4	13.3	21.0	20.5	5.00	4.913
4.0	31.3	31.1	93.3	92.1	9.00	8.913
8.0	81.7	81.4	472.	469.	17.0	16.91
16.0	233.	—	2640	—	33.0	—
32.0	713.	—	15900	—	65.0	—
64.0	2290	—	101000	—	129.0	—
128.0	7660	—	673000	—	257.0	—
1000.0	315000	—	2.13×10^8	—	2000.	—

$$* \text{roughness} = \frac{\text{surface area of protrusion}}{\text{surface area of protrusion base}}$$

protrusion base) of the protrusions, is given in the table for comparison.

The effect of rounding the corners on the total dimensionless force is small. As one would expect, the difference is the greatest for the lowest-aspect-ratio protrusion ($h/a=0.1$ for the cylinders with the rounded corners), where the radius of curvature of the rounded corner is equal to the protrusion height. However, even for this aspect ratio, the total dimensionless force for the cylinder with the sharp corner is only 8% higher than for the cylinder with the rounded corner. This difference drops to about 2% for a protrusion with an aspect ratio of 1. However, if the total force per unit surface area of the protrusion is compared for the sharp and rounded corners, then one finds that the values agree to within 1% over the aspect ratio range between $h/a = 0.1$ to 8. The force per unit surface area of the protrusion is calculated by dividing the total dimensionless force by the roughness.

The total dimensionless disturbance force on the cylinders ($\bar{F}_y^p = (F_y/\pi\mu\kappa a^2) - 1$) is plotted against h/a in Figure 2.18 for cylinders with sharp corners. The disturbance force is zero when the protrusion height is zero. It appears that rate of increase in the disturbance force is approaching different asymptotic slopes at high and low aspect ratios, and the slopes both have not yet converged at the limits of the aspect ratio range. The slopes at the extreme limits are 0.826 for the low aspect ratios and 1.81 for the high aspect ratios. The aspect ratio where these two lines intersect is approximately 3.

To determine whether these slopes are reasonable, the following intuitive argument is posed. On a constant radius basis, one might expect the local disturbance force on the protrusion to increase in proportion to x/a since the velocity increases linearly with distance from the surface. On top of the protrusion, x/a is a constant, and on the sides x/a linearly increases. After integrating over the surface of the protrusion, the total dimensionless disturbance force has the form $\bar{F}_y^p \sim c_1 (h/a) + c_2 (h/a)^2$, where c_1 and c_2 are constants. The first term contains the effect from the top of the protrusion, and the second term contains the effect from the side of the protrusion. At low aspect ratios, the first term dominates and the slope on a log-log plot is 1. At high aspect ratios the second term dominates, and the slope on a log-log plot is 2. The actual slopes of 0.826 and 1.81

Figure 2.18: The total dimensionless disturbance force as a function of aspect ratio for cylindrical protrusions with sharp corners.

Table 2.4: The total force on cylindrical protrusions with sharp corners compared to the total force on the side and the top of the same cylinders for various aspect ratios. The columns for $F_y^{\text{top}}/\pi\mu\kappa a^2$ and $F_y^{\text{side}}/\pi\mu\kappa a^2$ contain unrounded numbers.

h/a	$F_y/\pi\mu\kappa a^2$	$F_y^{\text{top}}/(\pi\mu\kappa a^2)$	$F_y^{\text{side}}/(\pi\mu\kappa a^2)$
0.01	1.08	1.037	0.045
0.05	1.31	1.165	0.144
0.1	1.57	1.282	0.291
0.2	2.08	1.484	0.600
0.3	2.60	1.663	0.933
0.4	3.12	1.829	1.288
0.5	3.65	1.945	1.709
0.6	4.20	2.090	2.111
0.65	4.48	2.150	2.330
0.7	4.76	2.240	2.524
0.8	5.34	2.319	3.021
0.9	5.93	2.442	3.490
1	6.54	2.85	3.69
1.5	9.80	3.238	6.567
2	13.4	3.720	9.709
4	31.3	5.755	25.58
8	81.7	9.135	72.59
16	233.	19.655	213.50
32	713.	35.78	677.22
64	2290	69.40	2224.8
128	7660	126.97	7537.72
1000	315000	1080.8	313916.8

are reasonably close to these values.

Because the above is just an intuitive argument, the asymptotic slopes are not required to be 1 and 2. However, it is interesting to note that the total dimensionless force on the top of cylindrical protrusions increases as h/a at the higher aspect ratios (where $\bar{F}_y^{\text{p}} \approx F_y/(\pi\mu\kappa a^2)$). This can be seen in Table 2.4 where the total dimensionless force on cylindrical protrusions are compared to the total dimensionless forces on the top and on the sides of the same cylinders. The values for the force on the top and the sides of the cylinders are unrounded, and these values are not as accurate as the total dimensionless force.

To take advantage of the axis of symmetry, the total dimensionless torque, T_z , was

calculated about the origin even though the protrusion would not rotate about this point if it was to tip over. Instead, it would rotate about the point $(x = 0, y = a, \phi = 0)$. The torque about the origin is probably a good approximation for the torque about the point $(x = 0, y = a, \phi = 0)$ for higher-aspect-ratio protrusions.

The total dimensionless torque is plotted against h/a in Figure 2.19 for cylinders with sharp corners. Both the torque and the aspect ratio are zero when h is zero. Similar to Figure 2.18, there appear to be two asymptotic slopes at the extreme limits of the aspect ratio range (1.26 at low h/a and 2.80 at high h/a), and the slopes have not yet converged. The change in the rate of increase in the torque occurs at about $h/a=2.3$, a slightly lower value than observed in Figure 2.18.

Another intuitive argument is posed to determine whether these slopes are reasonable. On top of the protrusion, the main contribution to the torque is expected to be from the shear stress, and on the side of the protrusion, the main contribution is expected to be from the normal force. The lever arm that is perpendicular to these forces is proportional to x/a . At low aspect ratios, the torque is dominated by the shear stress on top of the protrusion, and the shear stress will be on the order of unity. Hence the total torque is expected to be on the order of h/a . At high aspect ratios, the total torque will be dominated by the normal force on the side of the protrusion, which is expected to be proportional to x/a . Hence, the local torque is expected to be proportional to $(x/a)^2$, and the integrated total torque is expected to be proportional to $(h/a)^3$. The expected slopes for the low- and high-aspect-ratio limits are 1 and 3, respectively, which are close to the observed slopes of 1.26 and 2.80.

2.11 Comparisons between protrusions of different geometries

For cylindrical protrusions, the extent of the wall shear-stress disturbance was discussed in Section 2.9, and the total dimensionless force was presented in Section 2.10.

Figure 2.19: The total dimensionless torque as a function of aspect ratio for cylindrical protrusions with sharp corners.

For a protrusion of non-cylindrical geometry, one might expect the disturbance to be similar to the disturbance caused by a cylindrical protrusion when total force on the individual protrusions is the same. In Table 2.5, the extent of the shear-stress disturbance on the wall is

Table 2.5: The extent of the wall-shear-stress disturbance for protrusions of different geometries. The same total dimensionless force, $F_y/\pi\mu\kappa a^2 = 4.30$, is exerted on each of the protrusions. The protrusions are a cylinder ($h/a = 0.618$), a hemisphere ($h/a = 1.$), and a cone ($h/a = 1.535$).

	The $ y /a$ values downstream or upstream of the protrusion corresponding to the given shear stress				The $ z /a$ values to either side of the protrusion corresponding to the given shear stress			
	$ \tau_w /\tau_w^\infty$				$ \tau_w /\tau_w^\infty$			
	0.8	0.9	0.95	0.98	0.8	0.9	0.95	0.98
cylinder $h/a = 0.618$	2.62	3.28	4.11	5.55	1.42	1.63	1.86	2.22
hemisphere $h/a = 1$	2.62	3.37	4.29	5.86	1.37	1.57	1.80	2.17
cone $h/a = 1.535$	2.64	3.47	4.49	6.21	1.22	1.40	1.61	1.95

compared for a cylindrical protrusion ($h/a = 0.618$), a hemispherical protrusion ($h/a = 1$), and a cone ($h/a = 1.535$). The total dimensionless force on each protrusion is 4.30. The cone, which has the largest aspect ratio, causes the greatest disturbance in the flow direction and the smallest disturbance in the transverse direction. In contrast, the cylinder, which has the smallest aspect ratio, causes the greatest disturbance in the transverse direction and the smallest disturbance in the flow direction. However, up to $|\tau_w|/\tau_w^\infty = 0.95$, the extents of the disturbance along both axes are within 12% of each other for the different geometries. This implies that, for protrusions with the same total dimensionless force but different geometries, the extent of the disturbance is similar, and that small differences in the disturbance in the flow direction is compensated by small differences of the opposite nature in the transverse direction.

The reason for this becomes apparent upon doing a force balance beginning with

$$\nabla_i \sigma_{ij} = 0. \quad (2.57)$$

Integrating equation 2.57 over some control volume and applying the divergence theorem, results in

$$\int_V \nabla_i \sigma_{ij} dV = \int_D \sigma_{ij} n_i dS = 0. \quad (2.58)$$

Now, the stress tensor, σ_{ij} , is written as the sum of the disturbance stress tensor, σ_{ij}^D , and the stress tensor for the undisturbed flow, σ_{ij}^∞ :

$$\sigma_{ij} = \sigma_{ij}^\infty + \sigma_{ij}^D. \quad (2.59)$$

Replacing σ_{ij} with σ_{ij}^D on the right side of equation 2.58 and splitting the integral over D into integrals over the surfaces D_p , D_w , and D_i , one obtains

$$\int_{D_p} \sigma_{ij}^D n_i dS + \int_{D_w} \sigma_{ij}^D n_i dS + \int_{D_i} \sigma_{ij}^D n_i dS = 0, \quad (2.60)$$

where the control volume shown in Figure 2.2 is used. In the above equation, the integral over the surface at infinity D_i is zero because the stress tensor, σ_{ij}^D , decreases as $1/r^3$ as shown in Appendix A.7.

Now, the force balance for σ_{ij}^∞ is written for hypothetical flow domain 2 (see Figure 2.2). The force balance is

$$\int_{D_b} \sigma_{ij}^\infty n_i dS - \int_{D_p} \sigma_{ij}^\infty n_i dS = 0, \quad (2.61)$$

where the negative sign arises because the normal vector on D_p points outside of this domain. Subtracting 2.61 from 2.60 gives

$$\int_{D_p} \sigma_{ij} n_i dS + \int_{D_w} \sigma_{ij}^D n_i dS - \int_{D_b} \sigma_{ij}^\infty n_i dS = 0 \quad (2.62)$$

where σ_{ij}^D and σ_{ij}^∞ were combined for the integral over D_p using equation 2.59. The integral over D_b is simply

$$\int_{D_b} \sigma_{ij}^\infty n_i dS = \kappa \mu A_b \quad (2.63)$$

Figure 2.20: A schematic of a protrusion which is nearly cylindrical, with a height-to-radius ratio of h/a , except a small portion is missing near the wall.

where A_b is the area of the protrusion base.

A_b is not necessarily the same as πa^2 . This is illustrated in Figure 2.20 which shows a protrusion which is nearly cylindrical except for the small portion missing near the base. In this case, the area of the protrusion base, A_b , is smaller than the projected area of the protrusion onto the wall, πa^2 . For cylindrical protrusions, cones, hemispheres, *etc.*, $A_b = \pi a^2$, but for a sphere touching a wall, for example, $A_b = 0$, and πa^2 is equal to the projected area of the sphere on the wall.

Normalizing the integrals in equation 2.62 with $\kappa\mu\pi a^2$ and simplifying the integral over D_b with equation 2.63 results in

$$\bar{F}_j = \frac{A_b}{\pi a^2} + \bar{F}_j^v \quad (2.64)$$

where

$$\bar{F}_j = \frac{\int_{D_p} \sigma_{ij} n_i dS}{\kappa\mu\pi a^2} \quad (2.65)$$

is the dimensionless force on the protrusion and

$$\bar{F}_j^v = -\frac{\int_{D_w} \sigma_{ij}^v n_i dS}{\kappa\mu\pi a^2} \quad (2.66)$$

is the negative of the dimensionless disturbance force on the wall ($\bar{F}_j$ and $\bar{F}_j^v > 0$). In the limit of zero protrusion height, $\bar{F}_j^v$ goes to zero and $A_b/\pi a^2$ must be unity because $\bar{F}_j$

must be unity. Equation 2.64 states that the total dimensionless force on the protrusion is different from the magnitude of the disturbance force on the wall by a ratio of areas. As mentioned in the introduction, O'Neill [30] found that the total force on a sphere touching a plane wall was equal and opposite to the total disturbance force on the wall. Our results agree with this conclusion since the ratio of areas is zero in this case.

The extent of the shear-stress disturbance for the cylindrical, hemispherical, and conical protrusions is re-examined now. For these geometries, the ratio of areas is one. As a result, the relation between the disturbance force and the total force is the same in each case. In light of this, it is not surprising that the extent of the wall disturbance is similar for these geometries. One might question whether similar comparisons could be made when the ratio of the areas is not the same.

To determine the validity of such comparisons, the nearly-cylindrical protrusion in Figure 2.20 is examined once again. The missing portion of the cylinder near the wall can be thought of as a small crevice. The total force on a cylinder with a crevice will be nearly identical to the total force on the corresponding cylinder without a crevice because the geometries are nearly identical. However, the magnitude of the total disturbance force on the wall will be different by about 1 because the ratio of areas is different by about 1. Since the velocities will be very low in the crevice region, the contribution to $\bar{F}_j^D$ from the crevice will be approximately unity. Hence, the disturbance force on the surface beyond the projection of the protrusions will be nearly identical for the two geometries, and, as a result, the extent of the shear-stress disturbance will also be nearly identical. This indicates that, when the disturbance extent for protrusions with different $A_b/\pi a^2$ is compared, one should compare protrusions on a constant total force basis, not on a constant disturbance force basis, as long as the difference in areas is due to a "crevice."

In Table 2.6, the disturbance extent is compared for a cylinder ($h/a = 1.56$), a sphere just touching a wall ($h/a = 2$), and a cone ($h/a = 2.97$); the total dimensionless force exerted on each protrusion is 10.2. The area ratio is equal to 1 for the cylinder and the cone and 0 for the sphere. One can think of the sphere touching the wall as

Table 2.6: The extent of the wall shear-stress disturbance for protrusions of different geometries. The same total dimensionless force, $F_y/\pi\mu\kappa a^2 = 10.2$, is exerted on each of the protrusions. The protrusions are a cylinder ($h/a = 1.56$), a sphere touching a wall ($h/a = 2$), and a cone ($h/a = 2.97$).

	The $ y /a$ values downstream or upstream of the protrusion corresponding to the given shear stress				The $ z /a$ values to either side of the protrusion corresponding to the given shear stress			
	τ_w/τ_w^∞				τ_w/τ_w^∞			
	0.8	0.9	0.95	0.98	0.8	0.9	0.95	0.98
cylinder $h/a = 1.56$	4.27	5.53	7.07	9.69	1.63	1.97	2.34	2.90
sphere $h/a = 2$	4.30	5.64	7.26	10.0	1.59	1.98	2.39	2.99
cone $h/a = 2.97$	4.22	5.69	7.46	10.4	1.39	1.65	1.97	2.47

having a crevice around its base. The extent of the disturbance is similar for the different geometries. Similar to the comparisons in Table 2.5, the extent of the disturbance in the flow direction monotonically increases with increasing aspect ratio. However, unlike the previous comparisons, the extent of the disturbance in the transverse direction does not monotonically decrease with increasing aspect ratio. Hence, if protrusions are compared on a constant total force basis, the highest-aspect-ratio protrusion will not always have the greatest flow-direction disturbance and the smallest transverse-direction disturbance, although this tends to be the case.

2.12 Singular points and flow topology

During the generation of streamlines and skin-friction lines, singular points are often encountered. Singular points occur where all components of the wall stress go to zero on a surface or where all components of the velocity go to zero in the fluid (as opposed to

stagnation points which are on the fluid boundaries only). Singular points were found only in the xy -plane. The purpose of this section is to understand the behavior of skin-friction lines and streamlines in the vicinity of a singular point.

As a means to this end, it is useful to examine equations of the general form

$$\begin{aligned}\frac{d\xi}{dt} &= F_\xi(\xi, \eta) \\ \frac{d\eta}{dt} &= F_\eta(\xi, \eta)\end{aligned}\tag{2.67}$$

where

$$F_\xi(\xi_0, \eta_0) = F_\eta(\xi_0, \eta_0) = 0\tag{2.68}$$

and (ξ_0, η_0) is a singular point. It is assumed that F_ξ and F_η and their first derivatives are continuous across the singular point. Equations 2.67 are intended to be analogous to equations 2.45 or 2.47, used for generating streamlines or skin-friction lines.

Expanding equation 2.67 in a Taylor series, applying condition 2.68, and keeping only the first-order terms results in

$$\begin{aligned}\frac{d\xi}{dt} &= \frac{dF_\xi(\xi_0, \eta_0)}{d\xi}(\xi - \xi_0) + \frac{dF_\xi(\xi_0, \eta_0)}{d\eta}(\eta - \eta_0) \\ \frac{d\eta}{dt} &= \frac{dF_\eta(\xi_0, \eta_0)}{d\xi}(\xi - \xi_0) + \frac{dF_\eta(\xi_0, \eta_0)}{d\eta}(\eta - \eta_0).\end{aligned}\tag{2.69}$$

which can be written in the simplified form

$$\begin{bmatrix} \frac{d\xi}{dt} \\ \frac{d\eta}{dt} \end{bmatrix} = \begin{bmatrix} A & B \\ C & D \end{bmatrix} \begin{bmatrix} \hat{\xi} \\ \hat{\eta} \end{bmatrix}\tag{2.70}$$

where A , B , C , and D are constants, $\hat{\xi} = \xi - \xi_0$, and $\hat{\eta} = \eta - \eta_0$. Equations, identical in form to 2.70, for generating skin-friction and streamlines lines, will be provided after the general properties of equation 2.70 have been explored.

A wide variety of singular points can be generated for different values of A , B , C , and D . Except for case 2.b below, the different types of singular points can be classified by using only three parameters, the determinant (Det), the trace (Tr), and discriminant (Dis)

of the matrix

$$\begin{bmatrix} A & B \\ C & D \end{bmatrix} \quad (2.71)$$

where

$$\begin{aligned} \text{Det} &= AD - BC \\ \text{Tr} &= A + D \\ \text{Dis} &= \text{Tr}^2 - 4\text{Det}. \end{aligned} \quad (2.72)$$

Using these parameters, the singular points are classified below in the same manner as Hunt *et al.* [39] (except for slight differences in terminology and for 2.b):

1. $\text{Det} < 0$, Saddle point
2. $\text{Det} > 0$, Nodal point
 - (a) $\text{Dis} > 0$, Regular node
 - (b) $\text{Dis} = 0$ and $B = C$, Radial node
 - (c) $\text{Dis} < 0$, Focal point
 - i. $\text{Tr} \neq 0$, Regular focal point
 - ii. $\text{Tr} = 0$, Center

Two additional cases ($\text{Det} = 0$; $\text{Det} > 0$, $\text{Dis} = 0$, $B \neq C$) are in Kaplan [40, Chapter 11]. The different types of singular points are shown in Figures 2.21 to 2.25.³ In each of these figures, the flow paths are reversed by multiplying the right side of equation 2.70 by -1. Also, lines AA and BB in Figures 2.21 and 2.22 are perpendicular only if $B = C$. We observe all of the above cases in the form of either skin-friction lines or streamlines in our numerical results, and, as discussed later, we know the conditions under which each of the above occur for axisymmetric geometries.

³Lighthill [37, Section 2.6] made further distinctions among different types of regular nodes by drawing vortex lines together with his skin-friction lines. Vortex lines are perpendicular everywhere to skin-friction lines and are tangent to the local vorticity vector.

Figure 2.21: A saddle point of separation ($\text{Tr} < 0$). The spacing of the flow trajectories becomes narrower as the trajectories approach line BB.

Figure 2.22: A regular node of separation ($\text{Tr} < 0$). Every trajectory except trajectory AA becomes tangent with trajectory BB close to the singularity.

Figure 2.23: A radial node of separation ($\text{Tr} < 0$). The flow trajectories are not tangent to any line.

Figure 2.24: A regular focus of separation ($\text{Tr} < 0$). The trajectory spirals an infinite number of times around the origin as the singularity is approached; yet the total length along the trajectory is finite. A focus is a type of node.

Figure 2.25: A center ($\text{Tr}=0$). It is neither a point of separation or attachment. A center is a type of node, and it is a subclass of a focal point.

In the above classifications, singular points are grouped into two main types by the sign of the determinant. When the determinant is negative, a saddle point arises, and when the determinant is positive, a nodal point arises. Nodal points are further subclassified into regular nodes if the discriminant is greater than 0, radial nodes if the discriminant is equal to zero, and foci if the discriminant is less than 0. Foci are subclassified into regular focal points if the trace is not equal to zero and centers if the trace is equal to zero.

Singular points can be points of separation, points of attachment, or, in the case of centers, neither. This distinction is made only for skin-friction lines. The singular points in Figures 2.21 to 2.24 are all points of separation. Take the regular node in Figure 2.22 as an example. As the skin-friction lines approach the node, they become more narrowly spaced along line BB, and there is progressively less room for the fluid. Hence, the fluid must move away from or separate from the boundary. Line BB is the “line of separation” associated with the regular nodal point of separation because other skin-friction lines become tangent

to it. Similarly, the saddle point in Figure 2.21 is a point of separation because the skin-friction lines become more narrowly spaced as they approach the trajectories along BB (the line of separation for this case). There are no lines of separation associated with the radial nodal point or the focal point of separation in Figures 2.23 and 2.24. Mathematically, one can distinguish between points of separation and attachment by calculating the trace of matrix 2.71. As shown near the end of this section, the trace is negative for all points of separation, and positive for all points of attachment.

For streamlines, half-saddles and half-nodes, which occur on the fluid boundaries, also must be considered. A half-saddle and a half-node are shown in Figure 2.26 and are designated by S'_a and N'_s , respectively. The "a" stands for attachment, the "s" stands for separation, and the prime indicates that these are half-nodes and half-saddles. As shown later, streamlines cannot be generated in the vicinity of half-nodes and half-saddles by an equation of the form of 2.70 since second-order terms in the Taylor series expansion must be considered around these points. A nodal point, N , in the fluid is shown in Figure 2.26a, but a saddle point, S , is not shown in either figure because saddle points were not observed within the fluid.

For a simply connected protrusion on a plane wall (*i.e.*, our geometry), Hunt *et al.* showed that

$$\left(\sum_N + \frac{1}{2} \sum_{N'} \right) - \left(\sum_S + \frac{1}{2} \sum_{S'} \right) = 0 \quad (2.73)$$

where $\sum_N$ and $\sum_{N'}$ are the total number of nodes and half-nodes and $\sum_S$ and $\sum_{S'}$ are the total number of saddles and half-saddles. Since half-nodes and half-saddles do not occur for skin-friction lines, the relation simplifies to

$$\sum_N - \sum_S = 0. \quad (2.74)$$

Topological rules 2.73 and 2.74 raise an interesting question. How does the total number of singular points increase as the intersection between a cylindrical protrusion and the wall is approached? As discussed in Section 2.8, an infinite sequence of singular points

Figure 2.26: Singular points in the fluid and on the boundary. Cross sections of the fluid in the xy -plane are shown for (a) a nodal point, N , in the fluid and a half-saddle point of attachment, S'_a , on the wall and for (b) a half-nodal point of separation, N'_s , on the wall.

is expected very close to this intersection in the xy plane; yet the above topological rules must be obeyed. For these topological rules to be useful, "sets" of singular points must be considered so that their total number satisfies equation 2.73 or 2.74. Furthermore, for skin-friction lines on cylindrical protrusions, one might expect that equation 2.74 must be satisfied on the protrusion and the wall separately since the skin-friction lines on the protrusion are isolated from the skin-friction lines on the wall by a 90° corner. When streamlines and skin-friction lines are examined in Sections 2.14 and 2.15, the topological rules are not satisfied in some cases because complete "sets" of singular points are not always resolved.

The equations for skin-friction lines that are analogous to equations 2.70 are examined now. For these equations, the singular points are assumed to occur only in the xy -plane. Hence, the singular point is given by $(x_0, \sigma_0, \phi_0 = 0^\circ)$ on the downstream side of the cylinder and by $(x_0, \sigma_0, \phi_0 = 180^\circ)$ on the upstream side of the cylinder. The equations are derived using equations 2.47, A.12, and A.13. The equations for the skin-friction lines near a singular point on the side of a cylinder are

$$\begin{aligned} \begin{bmatrix} \frac{d(\hat{x}/\sigma_0)}{dt} \\ \frac{d\phi}{d(\kappa t)} \end{bmatrix} &= \pm \begin{bmatrix} \frac{\hat{\sigma}}{\kappa\mu} \frac{d\mathfrak{F}_x}{dx} & 0 \\ 0 & -\frac{\hat{\sigma}}{\kappa\mu\sigma_0} \mathfrak{F}_\phi \end{bmatrix} \begin{bmatrix} \hat{x}/\sigma_0 \\ \phi \end{bmatrix} \\ &= \pm \begin{bmatrix} \frac{1}{\kappa} \frac{d\mathcal{U}_{xl}}{dx} & 0 \\ 0 & -\frac{1}{\kappa} \frac{\mathcal{U}_{\phi l}}{\sigma_0} \end{bmatrix} \begin{bmatrix} \hat{x}/\sigma_0 \\ \phi \end{bmatrix}, \end{aligned} \quad (2.75)$$

and, for a singular point on the wall or the top of a cylinder, the equations are

$$\begin{aligned} \begin{bmatrix} \frac{d(\hat{\sigma}/\sigma_0)}{dt} \\ \frac{d\phi}{d(\kappa t)} \end{bmatrix} &= \pm \begin{bmatrix} \frac{\hat{x}}{\kappa\mu} \frac{d\mathfrak{F}_\sigma}{d\sigma} & 0 \\ 0 & -\frac{\hat{x}}{\kappa\mu\sigma_0} \mathfrak{F}_\phi \end{bmatrix} \begin{bmatrix} \hat{\sigma}/\sigma_0 \\ \phi \end{bmatrix} \\ &= \pm \begin{bmatrix} \frac{1}{\kappa} \frac{d\mathcal{U}_{\sigma l}}{d\sigma} & 0 \\ 0 & -\frac{1}{\kappa} \frac{\mathcal{U}_{\phi l}}{\sigma_0} \end{bmatrix} \begin{bmatrix} \hat{\sigma}/\sigma_0 \\ \phi \end{bmatrix}, \end{aligned} \quad (2.76)$$

where the positive signs are used when $\phi = 0^\circ$ (downstream) and the negative signs are

used when $\phi = 180^\circ$ (upstream). The quantities in each matrix position are dimensionless. Also, since these equations were derived specifically for a cylindrical protrusion, $\hat{\sigma}$ is positive in equation 2.75 and $\hat{x}$ is positive in equation 2.76. The subscript l on $\mathfrak{U}_{\sigma l}$ and $\mathfrak{U}_{\phi l}$ indicates that these terms are evaluated in the limit of very small distances from the surface.

Some immediate conclusions can be made from equations 2.75 and 2.76 because the cross terms B and C are equal to zero. First, for saddle points and regular nodes, the trajectories corresponding to lines AA and BB in Figures 2.21 and 2.22 must be perpendicular. Second, if the A term is equal to the D term, then a radial node will result. In Section 2.15, it is shown that such a node will occur for an h/a between 0.5 and 2.0. Third, the discriminant must be greater than or equal to zero. Hence, both regular foci and centers cannot occur as skin-friction lines. These results apply for three-dimensional flow around axisymmetric geometries in general except, possibly, when a singular point on the boundary lies on the axis of symmetry. In this case, all first derivatives in the shear stress are zero, and one must consider second-order terms to elucidate the behavior around the singularity. Such a case arises in shear flow over an axisymmetric cylindrical pit for a height-to-radius ratio between 0.25 and 1.0 (see Pozrikidis [41]).

More conclusions can be drawn if $\mathfrak{F}_\phi$ is always positive (*i.e.*, $D < 0$ downstream and $D > 0$ upstream), as was found to be the case to the resolution limit of our calculations. As a result, when $d\mathfrak{F}_x/dx$ or $d\mathfrak{F}_\sigma/d\sigma$ is negative, the determinant is positive (both upstream and downstream), and a nodal point arises. Similarly, if these derivatives are positive, a saddle point arises. The sign of the derivatives is presumed to alternate an infinite number of times as the intersection between the protrusion and the wall is approached, corresponding to an infinite sequence of Moffatt eddies. This implies that there will be an infinite sequence of saddle points and nodes in the skin-friction lines.

Also, if $\mathfrak{F}_\phi$ is always positive, every node at $\phi = 0^\circ$ (downstream) will be a nodal point of separation, and every node at $\phi = 180^\circ$ (upstream) will be a nodal point of attachment. In general, a point of separation on the downstream side of the protrusion is a point of attachment at the corresponding singularity upstream of the protrusion, whether

it is a saddle point or a node. To determine whether a saddle point is a point of attachment or separation, one needs to calculate the "A/D ratio." If $0 > A/D > -1$, then $\text{Tr} < 0$ at $\phi = 0$ and $\text{Tr} > 0$ at $\phi = 180$. Hence, it is a separation point downstream and an attachment point upstream. If $A/D < -1$, then $\text{Tr} > 0$ at $\phi = 0$ and $\text{Tr} < 0$ at $\phi = 180$. Hence, it is an attachment point downstream and a separation point upstream. The "A/D ratio" is

$$A/D = -\sigma_0 \frac{d\mathfrak{F}_x}{dx} / \mathfrak{F}_\phi \quad (2.77)$$

on the side of the protrusion and

$$A/D = -\sigma_0 \frac{d\mathfrak{F}_\sigma}{d\sigma} / \mathfrak{F}_\phi \quad (2.78)$$

on the wall or on top of the protrusion. For a nodal point, the ratio is always positive, and for a saddle point, the ratio is always negative.

To show that a singular point is, indeed, a point of separation if the trace is less than zero and a point of attachment if the trace is greater than zero, the continuity equation is employed. For axisymmetric geometries, the continuity equation reduces to

$$\begin{aligned} \frac{d\mathfrak{U}_x}{dx} + \frac{1}{\sigma} \frac{d\sigma \mathfrak{U}_\sigma}{d\sigma} + \frac{\mathfrak{U}_\sigma}{\sigma} - \frac{\mathfrak{U}_\phi}{\sigma} \\ = \frac{d\mathfrak{U}_x}{dx} + \frac{d\mathfrak{U}_\sigma}{d\sigma} + \frac{\mathfrak{U}_\sigma}{\sigma} - \frac{\mathfrak{U}_\phi}{\sigma} = 0, \end{aligned} \quad (2.79)$$

where the equation is applicable both upstream and downstream of the cylinder because the ϕ dependence can be eliminated without defining the location of the singular points. For very small distances from the singularity, $\frac{d\mathfrak{U}_\sigma}{d\sigma} \gg \frac{\mathfrak{U}_\sigma}{\sigma}$, and equation 2.79 reduces to

$$\frac{d\mathfrak{U}_{xl}}{dx} + \frac{d\mathfrak{U}_{\sigma l}}{d\sigma} - \frac{\mathfrak{U}_{\phi l}}{\sigma_0} = 0, \quad (2.80)$$

where σ has been approximated by σ_0 . The following analysis is done for a singular point on the side of a cylinder and for $\phi_0 = 0^\circ$ or 180° . Equating the traces of the matrices in equation 2.75 yields

$$\frac{1}{\mu} \left(\frac{d\mathfrak{F}_x}{dx} - \frac{\mathfrak{F}_\phi}{\sigma_0} \right) \hat{\sigma} = \frac{d\mathfrak{U}_{xl}}{dx} - \frac{\mathfrak{U}_{\phi l}}{\sigma_0}. \quad (2.81)$$

Replacing $d\sigma$ in equation 2.80 with $d\hat{\sigma}$, substituting equation 2.81 into equation 2.80, and integrating results in

$$\begin{aligned}\mathcal{U}_{\sigma l} &= -\frac{1}{\mu} \left(\frac{d\mathfrak{F}_x}{dx} - \frac{\mathfrak{F}_\phi}{\sigma_0} \right) \frac{\hat{\sigma}^2}{2} \\ &= -\Delta \frac{\hat{\sigma}^2}{2}\end{aligned}\quad (2.82)$$

where $\text{Tr} = \Delta\hat{\sigma}$, Tr is the trace of equation 2.75, and $\hat{\sigma}$ is positive. As a result, if $\text{Tr} < 0$, then $\Delta < 0$ and $\mathcal{U}_{\sigma l} > 0$. In other words, the singular point must be a point of separation. A similar equation could be derived for $\mathcal{U}_{xl}$ if the singularity is on the wall or on the top of the cylinder. In general, the velocity normal to the surface increases as the square of the distance from the surface, which agrees with Lighthill's analysis of skin-friction lines [37, page 72]. A consequence of this is that streamlines cannot be generated in the vicinity of half-nodes and half-saddles by an equation of the form 2.70 because second-order terms in the Taylor series expansion must be considered around these points.

The differential equations corresponding to 2.70 for streamline generation in the vicinity of a singular point in the fluid are

$$\begin{bmatrix} \frac{dx}{dt} \\ \frac{d\sigma}{dt} \end{bmatrix} = \pm \begin{bmatrix} \frac{d\mathcal{U}_x}{dx} & \frac{d\mathcal{U}_x}{d\sigma} \\ \frac{d\mathcal{U}_\sigma}{dx} & \frac{d\mathcal{U}_\sigma}{d\sigma} \end{bmatrix} \begin{bmatrix} \hat{x} \\ \hat{\sigma} \end{bmatrix}, \quad (2.83)$$

where the plus sign is for $\phi = 0^\circ$ and the negative sign is for $\phi = 180^\circ$. Equation 2.83 is in dimensional form. For saddle points and regular nodes, the trajectories corresponding to lines AA and BB in Figures 2.21 and 2.22 must not be perpendicular since B must not be equal to C . However, we did not observe saddle points within the fluid (half-saddles, of course, occur on the boundary), but it is not apparent from equation 2.83 that the determinant cannot be less than zero. Another consequence of $B \neq C \neq 0$ is that the discriminant can be less than zero, and regular foci can occur; regular foci were observed in our results. However, unless the singularity occurs on the axis of symmetry, we assert that centers (or closed streamlines) cannot exist in the flow, as the following physical argument suggests. For closed streamlines to exist, the trace of equation 2.83 must be zero. Then, by equation 2.80 (the l subscripts in equation 2.80 are dropped), $\mathcal{U}_\phi$ must also be zero.

Since $u_\phi = -\sin(\phi)\mathcal{U}_\phi$ (from equation A.12), there must be a ring of stagnation points lying in a circle around the protrusion. This seems unlikely to occur even under exceptional circumstances. However, if the center were on the axis of symmetry, closed streamlines would occur. Pozrikidis [41] found closed streamlines when a singular point was located on the axis of symmetry for three-dimensional creeping flow in axisymmetric cavities or orifices. Also, Hunt *et al.* [39] asserted that closed streamlines cannot occur in viscous three-dimensional flows for any finite Reynolds number.

2.13 Side, top, front, and isometric views of streamlines around a cylindrical protrusion, $h/a = 1$

An isometric projection of streamlines around a cylindrical protrusion ($h/a = 1$) is shown in Figure 2.27 to illustrate the three-dimensional nature of the flow. Also, included in the figure are side, top, and front views of the flow trajectories. Since the flow is symmetric about the xz and xy planes, only one quarter of the protrusion geometry is shown. For each view, the flow trajectories are marked with a 1, 2, or 3. Flow trajectory 1 originates at the greatest distance from the wall upstream of the protrusion, and flow trajectory 2 and 3 are at about the same distance from the wall. Trajectory 3, however, originates a little farther from the xy -plane than trajectory 2.

Trajectory 1 originates far enough away from the wall that it is simply swept over the protrusion, whereas trajectory 2 and 3 go around the protrusion. As 2 and 3 approach the protrusion, they first bend away from the wall, but very close to the protrusion, both trajectories dip toward the wall. Trajectory 3 never gets very close to the wall. Trajectory 2, on the other hand, approaches the wall closely, reverses flow direction, and then is swept around the protrusion. On the back side of the protrusion, taking trajectory 2 as an example, the fluid is swept the rest of the way around the protrusion, reverses flow direction in the wake, moves away from the wall along the protrusion, and then is swept downstream.

From the top view (c) and the front view (d), one can see that trajectory 2 origi-

Figure 2.27: 3-dimensional flow trajectories around a cylindrical protrusion with $h/a=1$. The views are: (a) isometric, (b) side, (c) top, and (d) front. The bold solid lines are the flow trajectories; the light solid lines outline 1/4 of the protrusion geometry. For each view, the flow trajectories are marked with a 1, 2, or 3. Upstream of the protrusion, flow trajectory 1 is at the greatest distance from the wall; flow trajectory 2 and 3 are at about the same distance from the wall, but trajectory 3 is a little bit further away from the symmetry plane.

nates very close to the xy -plane upstream of the protrusion. Trajectory 3, which originates only slightly farther away from the xy -plane, is swept around the protrusion without being caught in the flow reversal region. Hence, only a very small amount of fluid participates in flow reversal. As seen earlier, however, this is a function of aspect ratio (*cf.*, Figure 2.16, which shows the size of the back-flow region in the shear-stress contours.) From the side view (b), one can see that each trajectory first moves gradually away from the wall as the protrusion is approached from upstream. Trajectory 2 and 3 do not begin moving toward the wall until they are within approximately 0.3 radii from the protrusion.

2.14 Flow trajectories in the xy -plane around cylindrical protrusions

Figures 2.28, 2.29, and 2.30 show flow trajectories in the xy -plane for $h/a = 8, 2$, and 0.5 , respectively. The flow trajectories are given by the solid lines, and the asterisks mark the location of singular points. N designates a node, N'_a and N'_s designate half-nodes, S'_a and S'_s designate half-saddles, and the subscripts a and s stand for attachment and separation, respectively. For purposes of discussion, the flow goes from left to right in the figures. The bottom graphs in Figures 2.29 and 2.30 show an expanded view of the streamlines on the downstream side of the protrusion.

There are two half-saddles near the top of each protrusion. One streamline attaches to the upstream half-saddle, and one streamline separates from the downstream half-saddle. These two streamlines form a boundary in the xy -plane, dividing the fluid into an "upper region" and a "lower region." Trajectories in the upper region flow over the protrusion and those in the lower region terminate at or radiate from one or more singular points. This also occurs at $h/a=8$, although the singular points in the lower region could not be resolved. For every point of attachment on one side of the protrusion, there is a corresponding point of separation on the other side of the protrusion. Every half-node and half-saddle on the downstream side is a point of separation, and every half-node and half-saddle on the

Figure 2.28: Flow trajectories in the xy -plane for a cylindrical protrusion with a height-to-radius ratio, h/a , equal to 8. The solid lines are flow trajectories; the asterisks are singular points.

Figure 2.29: Flow trajectories in the xy -plane for a cylindrical protrusion with a height-to-radius ratio, h/a , equal to 2. The bottom graph is an expanded view of the recirculation region. The solid lines are flow trajectories; the asterisks are singular points.

Figure 2.30: Flow trajectories in the xy -plane for a cylindrical protrusion with a height-to-radius ratio, h/a , equal to 0.5. The bottom graph is an expanded view of the recirculation region. The solid lines are flow trajectories; the asterisks are singular points.

upstream side is a point of attachment, except at $h/a=0.5$ where there are two half-saddle points of attachment on the downstream side (S'_{a1} and S'_{a3}) and two half-saddle points of separation on the upstream side (S'_{s1} and S'_{s3}). Only single streamlines terminate at half-saddles, but multiple streamlines terminate at half-nodes and nodes.

At $h/a = 8$, the streamlines do not appear to reverse flow direction; at $h/a = 2$, the streamlines do reverse direction, but only very close to the wall; and at $h/a = 0.5$ the flow reversal is more noticeable. For $h/a = 2$ (taking the downstream side as an example) flow reversal occurs between S'_{s1} and N'_{s1} , and, for $h/a=0.5$, flow reversal occurs between S'_{s2} and S'_{a1} . Flow reversal also occurs between the corresponding nodes on the upstream side of the protrusion.

The number of singularities that are marked in each figure is insufficient to satisfy topological rule 2.73. To make up the difference, there are, presumably, more nodes closer to the intersection between the protrusion and the wall that could not be resolved. For example, at $h/a=8$, it is likely that the half-saddles on the protrusion are balanced by unresolved half-nodes on the wall very close to the protrusion. For $h/a=2$, the accounting also could be done by balancing singularities on the protrusion with singularities on the wall. On the downstream side, N'_{s1} on the wall balances S'_{s2} on the protrusion, and S'_{s1} on the wall is balanced by an unresolved half-node on the protrusion. The accounting is different at $h/a = 0.5$. Here, it appears that a half-saddle on the wall and a half-saddle on the protrusion balance a node in the fluid. On the downstream side, for example, this implies that there is an unresolved node in the fluid close to S'_{s2} and S'_{a3} .

Between $h/a=0.5$ and 2, the flow topology undergoes an interesting transition. At $h/a = 2$ and 8, there are no nodes in the fluid, but at $h/a=0.5$, a regular focal point is in the fluid. Upon further examination, singular points are found in the fluid for approximately $h/a \leq 0.8$. Below this aspect ratio, the half-node moves from the wall and into the fluid, where it becomes a regular node. At even lower aspect ratios, the singularity moves farther from the wall and becomes a regular focal point. Figure 2.31 shows expanded views of the singularities at different stages of the transition. A half-node is present at $h/a=1$, a regular

node is present at $h/a=0.7$, and a focus point is present at $h/a=0.5$. The scale on the ordinates shows that the singularity appears progressively farther from the wall at lower aspect ratios. At $h/a=0.7$, the regular node is at about $0.0565h$, and at $h/a=0.5$ the focal point is at about $0.136h$.

2.15 Skin-friction lines around cylindrical protrusions

Skin-friction lines are shown from a top view in Figures 2.32 to 2.34 for cylindrical protrusions of $h/a=8$, 2, and 0.5, respectively. The bottom plots in the figures show an expanded view of the skin-friction lines in the top plots. The two scales are the same for each aspect ratio. The nodal and saddle points are marked by an N or S , respectively. The subscripts "a" and "s" designate points of attachment and separation, respectively. Skin-friction lines on the side of these cylinders are shown in Figure 2.35. In this figure, the cylinders are unscrolled and laid flat, and only the downstream end is viewed, centered around $\phi = 0^\circ$.

On the upstream side of the protrusion, the first two singular points are a saddle point and a node in that order. For $h/a=8$, the saddle-node pair could not be resolved, but it presumably exists very close to the protrusion. On the downstream side of the protrusion, the saddle and node points occur in reverse order. A saddle and node are also the first two singularities typically uncounted for flow around protrusions at finite Reynolds numbers [42]. As discussed in Section 2.12, if $\mathfrak{F}_\phi$ is positive everywhere, then the singular points on the wall will alternate between saddles and nodes, satisfying topological rule 2.74 with each pair.

The skin-friction lines that intersect singular points coincide with line L or curves C in Figures 2.32 to 2.35. Line L runs along the surface in the xy plane. Curves C appear as circles in the top views and as horizontal lines in the "side views." The subscript n is used when C intersects a node, and s is used when C intersects a saddle. C and L intersect at right angles, and all of the nodal points are regular nodes, as predicted by the analysis

Figure 2.31: Expanded views of singular points in the fluid and on the wall for cylindrical protrusions of various aspect ratios. (a) $h/a = 0.5$, an expanded view of the focus in Figure 2.30 but only one streamline is shown; (b) $h/a = 0.7$, a regular node in the fluid; (c) $h/a = 1.0$, a half-node on the wall.

Figure 2.32: Skin-friction lines as viewed from above a cylindrical protrusion with a height-to-radius ratio, h/a , equal to 8. The bottom graph is an expanded view of the top graph.

Figure 2.33: Skin-friction lines as viewed from above a cylindrical protrusion with a height-to-radius ratio, h/a , equal to 2. The bottom graph is an expanded view of the top graph.

Figure 2.34: Skin-friction lines as viewed from above a cylindrical protrusion with a height-to-radius ratio, h/a , equal to 0.5. The bottom graph is an expanded view of the top graph.

Figure 2.35: Skin-friction lines on the side of cylindrical protrusions with height-to-radius ratios equal to $h/a = 0.5, 2$, and 8 . The solid lines are the skin-friction lines, the dashed lines mark the top boundary of the protrusions, and the asterisks mark the location of singular points.

in Section 2.12.

For the top views, the fluid reverses direction at each curve C . Because no C curve appears in Figure 2.32, no flow reversal is observed at $h/a=8$. At $h/a=2$ and 0.5 , flow reversal is observed between C_{s1} and C_{n1} both upstream and downstream of the protrusion, only close to line L at $h/a=2$ and over a broader area around line L for $h/a=0.5$. Also, at $h/a=8$, it is evident from the "side views" that the fluid does not move vertically toward or away from the wall to any significant degree. At higher aspect ratios, the fluid is mainly swept horizontally around the protrusion without flow reversal; yet the extent of the disturbance is larger at higher aspect ratios.

The circular skin-friction lines arise for the following reason. At a singular point $(x_0, \sigma_0, \phi=0)$, $f_x = \cos(\phi)\mathfrak{F}_x$ and $f_\sigma = \cos(\phi)\mathfrak{F}_\sigma$ are zero because $\mathfrak{F}_x$ and $\mathfrak{F}_\sigma$ are zero, but $f_\phi = \sin(\phi)\mathfrak{F}_\phi$ is zero only because $\sin(0)$ is zero. As a result, f_x and f_σ must be zero for all ϕ , but f_ϕ is not. It follows that a fluid parcel that lies adjacent to the surface along $(x_0, \sigma_0, 0 < \phi < 2\pi)$ must trace out a circular arc.

All skin-friction lines that originate from a nodal point on the upstream side of the protrusion terminate at a corresponding node on the downstream side of the protrusion. Skin-friction lines associated with a given pair of nodes are separated from other skin friction lines by one or more C_s curves. For example, the skin-friction lines associated with the pair of nodes near the top of each protrusion are isolated from other skin-friction lines by a C_s curve near the base of the protrusion. This curve corresponds to C_{s2} for $h/a=0.5$ in Figure 2.35. Presumably, such curves also exist for $h/a=2$ and 8 , but they are too close to the base of the protrusion to be resolved.

Because all nodal points are regular nodes for skin-friction lines, there must be tangent lines similar to BB in Figure 2.22, such as line L for $h/a=2$ and 8 and curve C_{n2} for $h/a=0.5$ in Figure 2.35. On the downstream side of the protrusion, this implies that L is a line of separation for $h/a=2$ and 8 and C_{n2} is a line of separation for $h/a=0.5$. The behavior of the skin-friction lines is mathematically verified in the vicinity of the node by calculating the A/D ratios discussed in Section 2.12. If the ratio is greater than 1, then

the skin-friction lines are tangent to one of the C curves, and if it is less than 1, then the skin-friction lines are tangent to line L . The ratios are 3.2, 0.87, and 0.19 for $h/a = 0.5$, 2, and 8, respectively, which is in accord with the observed behavior. If the A/D ratio is 1, then a radial node occurs, as should be the case for an aspect ratio somewhere between $h/a=0.5$ and 2.

Similar comparisons can be made for the skin-friction lines in the vicinity of saddle points. In the top views, for example, the skin-friction lines are tangent to L for $h/a=8$ and 2 and to curve C_{s1} for $h/a=0.5$. On the downstream sides of the protrusions, this implies that a line of separation coincides with L for $h/a=2$ and 8 and that a line of attachment coincides with C_{s1} for $h/a=0.5$. C_{s2} is a line of attachment because the skin-friction lines become more widely spaced with downstream distance. One can verify the tangents and determine whether the singularities are attachment or separation points for the saddle points by calculating the associated A/D ratios. For $A/D < -1$, the tangent is one of the C curves and the saddle is an attachment point for $\phi = 0^\circ$ (downstream) and a separation point for $\phi = 180^\circ$ (upstream). For $0 > A/D > -1$, the tangent is line L and the saddle is a separation point for $\phi = 0^\circ$ and an attachment point for $\phi = 180^\circ$. The A/D ratios for the nodes and saddles in Figures 2.32 to 2.35 are given in Table 2.7.

2.16 Flow trajectories around a hemispherical protrusion

Figure 2.36 shows the flow trajectories around a hemispherical protrusion. The total number of singularities in Figure 2.36 (top) satisfies topological rule 2.73. The bottom graph is a magnified view of two singular points in the wake, which are a regular nodal point in the fluid at $x/h = 0.0116$ and a half-saddle point of attachment on the wall. The flow separates from the hemisphere at $\theta = 73.2^\circ$, and the saddle point of attachment in the wake is at $y/a = 1.22$ —the same two values calculated by Price [31]. However, Price implied that flow trajectories connect the singular points on the protrusion to the singular points on the wall. As can be seen in Figure 2.36, this is not the case.

Figure 2.36: Flow trajectories in the xy -plane for a hemispherical protrusion. The bottom graph is an expanded view of the top graph near the singular point on the wall.

Table 2.7: The " A/D ratio" for the singular points in Figures 2.32 to 2.35. The A/D ratio is defined by equations 2.77 and 2.78.

h/a	Identifier	A/D ratio
0.5	S_{a1} (downstream)	-1.7
	S_{s1} (upstream)	
	S_{a2} (downstream)	< -1
	S_{s2} (upstream)	
	N_{s1} (downstream)	> 1
	N_{a1} (upstream)	
2	N_{s2} (downstream)	+3.2
	N_{a2} (upstream)	
	S_{s1} (downstream)	-0.26
	S_{a1} (upstream)	
	N_{s1} (downstream)	+0.17
	N_{a1} (upstream)	
8	N_{s2} (downstream)	+0.87
	N_{a2} (upstream)	
8	N_{s1} (downstream)	+0.19
	N_{a1} (upstream)	

2.17 Expected effects of the fluid flow on mass transport

Mass transport is discussed in Chapter 5 for an insulating cylindrical protrusion ($h/a \approx 0.8625$) on an active electrode surface. Although the Reynolds numbers are finite (the lower Reynolds numbers ranged from $Re_p = 0.56$ to 5), the general results are not surprising based on the expected behavior of the fluid in the limit of creeping flow. For example, mass transport is inhibited over distances of several protrusion radii around the protrusion because of a decrease in the shear stress at the wall. Close to the front of the protrusion, however, mass transport is enhanced because of convection toward the electrode (*i.e.*, the wall). In the immediate wake of the protrusion, the mass transport is the lowest because of the combined effect of electrolyte depletion and convection away from the wall. At $h/a = 0.8625$, the streamlines terminate at either a half-node or a half-saddle on the boundary.

2.18 Conclusions

The first nine conclusions concern flow separation and flow reversal. For these conclusions, one should keep in mind that for every separation point on the downstream side of the cylinder, there is a corresponding attachment point on the upstream side of the cylinder and *vice versa*. Also, for every flow-reversal region on the downstream side of the cylinder, there is a corresponding flow-reversal region on the upstream side of the cylinder.

1. Flow separation occurs when the protrusion and the wall intersected at angles less than approximately 124° . This is the same angle at which an infinite set of Moffatt eddies first appear in two-dimensional corners [38]. This implies that there may also be an infinite sequence of eddies in the xy plane when this critical angle is exceeded for axisymmetric protrusions. For cylindrical protrusions, flow separation is always observed since the angle of intersection, 90° , is less than the critical angle of 124° . However, flow reversal is not always detectable. At cylinder aspect ratios higher than an h/a between 2.4 and 2.6, no flow reversal is observed. At these high aspect ratios, however, it is possible that there are unresolvable Moffatt-like eddies very close to the protrusion.
2. Since flow reversal is observed in the limit of creeping flow, flow reversal occurs even for infinitesimally small protrusions.
3. In his paper on linear shear flow around a hemispherical protrusion, Price [31] implies that a streamline connects a singular point on the protrusion to a singular point on the wall. This is not observed in our study. When flow separates from the hemisphere, it does not re-attach to the wall farther downstream. This is generally true for other axisymmetric protrusion geometries.
4. For cylindrical protrusions, as the aspect ratio is increased, the recirculation region becomes narrower in the transverse direction, moves away from the protrusion, becomes weaker in strength, and extends farther in the flow direction. Then, somewhere

between h/a of 2.4 and 2.6, the recirculation region becomes smaller in both directions and completely disappears.

5. Flow separates near the top of cylindrical protrusions at all aspect ratios, and the separation point moves closer to the top of the protrusion at higher aspect ratios. At $h/a = 0.1$, the separation point is at $x/h = 0.864$. At $h/a = 8$, the separation point is at $x/h = 0.941$.
6. At high aspect ratios (*e.g.*, $h/a = 8$), fluid is swept around the protrusion with little vertical motion and without flow reversal (except, possibly, in undetectable Moffatt-like eddies). At lower aspect ratios (*e.g.*, $h/a = 2$ and 0.5), flow reversal is detectable, and the vertical motion of the fluid is more pronounced as it is swept around the protrusion.
7. At $h/a = 0.5$, the streamlines around the focal point in the fluid resemble the closed-streamline patterns in two-dimensional flow over square ridges [43]. One can think of a two-dimensional step as a protrusion with a finite height and an infinite radius of curvature. Hence, the appearance of the streamlines in the xy plane at small h/a is similar to the streamlines around a two-dimensional ridge.
8. On the downstream side of the cylinders, the flow separates from the protrusion along a line L perpendicular to the wall at $h/a = 2$ and 8 . At $h/a = 0.5$, the flow separates along a curve C , parallel to the wall near the top of the cylinder. The transition in the mode of separation occurs somewhere between $h/a = 0.5$ and 2 , where a radial node appears in the skin-friction lines. For a two-dimensional square ridge, the flow separates along a horizontal line parallel to the wall near the top of the protrusion [43]. This is more evidence that flow around axisymmetric protrusions with lower aspect ratios should appear similar to flow around two-dimensional ridges.
9. Unlike flow over two-dimensional ridges [43], closed streamline patterns are not observed in the recirculation patterns around axisymmetric protrusions. Closed stream-

lines are only observed when the fluid is trapped, such as in three-dimensional flow over axisymmetric cavities [41]. Hunt *et al.* [39] asserted that closed streamlines cannot occur in viscous three-dimensional flows for any finite Reynolds number.

The following conclusions are related to total dimensionless forces, total dimensionless torques, and/or the dimensionless wall shear-stress distribution.

1. The negative of the total dimensionless disturbance force on the wall ($\bar{F}_j^v > 0$) is related to the total dimensionless force on the protrusion ($\bar{F}_j > 0$) by $\bar{F}_j^v = A_b/\pi a^2 + \bar{F}_j$, where $A_b/\pi a^2$ is the ratio of the area of the protrusion base (A_b) to the projected area of the protrusion on the wall (πa^2). For a cylindrical protrusion, this ratio is 1, and, for a sphere touching a wall, this ratio is 0. This result agrees with O'Neill's conclusion for a sphere touching a wall [30].
2. When the same total dimensionless force is exerted on protrusions of different geometries and when $A_b/\pi a^2$ is the same for the different protrusions, the extent of the shear-stress disturbance on the wall is similar. Protrusions with higher aspect ratios tend to have a slightly larger flow direction disturbances and a slightly smaller transverse direction disturbances.
3. When the same total dimensionless force is exerted on protrusions of different geometries and when $A_b/\pi a^2$ is not the same for the different protrusions, the extent of the shear-stress disturbance on the wall is similar, as long as the difference in $A_b/\pi a^2$ is due to a small crevice near the base of the protrusion.
4. The total dimensionless disturbance force on cylindrical protrusions increases approximately as $(h/a)^{0.826}$ at low aspect ratios and as $(h/a)^{1.81}$ at high aspect ratios. The transition between these two regions occurs at about $h/a = 3$.
5. The total torque about the origin on cylindrical protrusions increases approximately as $(h/a)^{1.26}$ at low aspect ratios and as $(h/a)^{2.80}$ at high aspect ratios. The transition between these two regions occurs at about $h/a = 2.3$.

6. Sharp corners do not cause large disturbances in the flow even though the shear stress tends toward infinity in these places. This is because the total dimensionless force on a cylinder with sharp corners is not dramatically different from the total dimensionless force on a cylinder with rounded corners. As a result, the extent of the fluid-flow disturbance is approximately the same. The difference in the total force between cylindrical protrusions with sharp and rounded corners ($\tau_c = 0.1a$) is roughly proportional to the difference in surface areas.
7. For the cylindrical protrusions that were studied, the extent of the dimensionless wall-shear disturbance increases with increasing aspect ratio. The extent of the disturbance increases more rapidly in the flow direction than in the transverse direction, and, as a result, the shear-stress contours adopt a characteristic dumbbell shape.

The following conclusions are related to flow topology.

1. Only positive values of $\mathfrak{F}_\phi$ were calculated. If $\mathfrak{F}_\phi$ can be less than zero, it could only be less than zero very close to the intersection of the protrusion and the wall.
2. For skin-friction lines, when $\mathfrak{F}_\phi > 0$, adjacent singular points alternate between saddle points and nodal points. The node is a regular node or a radial node, as defined in Section 2.12. Each saddle-node pair satisfies topological rule 2.74. Upstream of the protrusion, the first two singular points are a saddle point and a node in that order. On the downstream side of the protrusion, the saddle and the node appear in reverse order. A saddle and a node are also the first two singularities typically encountered on the wall for flow around protrusions at finite Reynolds numbers [42].
3. All skin-friction lines which originate from a nodal point upstream of the protrusion terminate at a corresponding node on the downstream side of the protrusion. Skin-friction lines associated with a given pair of nodes are separated from other skin friction lines by one or more C_s curves.

4. For $h/a \geq 0.8$, the streamlines in the xy plane terminate at a half-node or half-saddle on the wall, or the streamlines are swept over the protrusion. At these aspect ratios, all half-saddles are separation points downstream of the protrusion and attachment points upstream of the protrusion. This is always true for half-nodes. One can mathematically verify whether a singularity is an attachment or separation point by calculating the " A/D ratio."
5. For $h/a \leq 0.8$, at least one of the half-nodes (and its counterpart on the other side of the protrusion) is a singular point in the fluid. First, the singularity becomes a regular node, and then, with further reduction in aspect ratio, the singularity becomes a focus. For example, at $h/a=0.7$, the singular point is a regular node, and, at $h/a=0.5$, the singular point is a regular focus. In place of the half-node that was on the wall, there is a half-saddle point of attachment on the wall downstream of the protrusion and a half-saddle point of separation on the wall upstream of the protrusion.
6. For streamlines, at $h/a \geq 0.8$, topological rule 2.73 appears to be satisfied by a half-saddle on the protrusion balancing a half-node on the wall or *vice versa*. At $h/a \leq 0.8$, topological rule 2.73 appears to be satisfied by one half-saddle on the protrusion and one half-saddle on the wall balancing a node in the fluid.
7. For streamlines, saddle points were not observed in our study. However, we were not able to prove that they could not occur in the fluid for three-dimensional flow around axisymmetric geometries. Half-saddles on the wall, of course, were observed.

Chapter 3

Experimental Apparatus and System Characterization

3.1 Introduction

A segmented microelectrode was designed and fabricated by us in the UC Berkeley Microfabrication Laboratory of Electrical Engineering and Computer Science (EECS) to measure local limiting currents in flowing electrolyte around single and multiple microscale polyimide protrusions. A flow cell for the limiting-current measurements was also designed and fabricated by us, but the electronic equipment used for taking the measurements was first assembled by Dennis Dees [44]. In the first half of this chapter, the microelectrode and the experimental apparatus are described, but the detailed fabrication procedure for the microelectrodes is not discussed until Appendix B. In the second half of this chapter, topics related to system characterization are discussed. System characterization includes the measurement of limiting-current curves, the determination of the background current distribution (*i.e.*, the current distribution with no protrusions), and a discussion of turbulent fluctuations. Turbulent fluctuations are discussed to explain why it was easier to determine mass-transport distributions in the direction of flow rather than in the transverse direction when the bulk fluid flow was turbulent.

Microfabricated electrodes were used for local mass-transport measurements by three previous researchers in our laboratory. Dees and Tobias [44] originally conceived and designed the so-called "micromosaic electrode." The microelectrodes in this design were $98\text{ }\mu\text{m}$ square and were arranged in a 10×10 array on $100\text{ }\mu\text{m}$ centers. The micromosaic electrodes were fabricated at Hewlett-Packard Laboratories. Dees used the micromosaic electrode to measure local mass-transport rates around growing, coalescing, and detaching hydrogen bubbles [44]. Whitney [45] used similar micromosaic electrodes (fabricated at Hewlett-Packard Laboratories and at AT&T Bell Laboratories) to measure the onset time for natural convection to occur at a horizontally oriented electrode. She also measured mass-transfer effects from a single rising hydrogen bubble column at a vertically oriented electrode. Sutija [5] redesigned and fabricated the micromosaic electrode at the UC Berkeley Microfabrication Laboratory. These microelectrodes were used to measure the mass-transport distribution resulting from multiple rising gas bubble columns at a vertically-oriented electrode. The arrangement of the microelectrodes in our design is significantly different from the arrangement of the microelectrodes in previous studies.

3.2 The segmented microelectrode, the flow cell, and the electronics

A scanning electron micrograph (SEM) of a segmented microelectrode (wafer 6) with a single protrusion is shown in Figure 3.1, and an SEM of a segmented microelectrode with a protrusion array (wafer 8) is shown in Figure 3.2. The SEMs were taken after completing all experiments with the individual devices. In each device, there are $22, 48.5\text{ }\mu\text{m} \times 48.5\text{ }\mu\text{m}$ square platinum microelectrodes embedded within, but electrically isolated from, a $0.5\text{ cm} \times 0.5\text{ cm}$ square platinum electrode (the "buffer electrode"). Most of the buffer electrode can be seen in Figure 3.2 (top). The microelectrodes are arranged in a cross pattern, and a polyimide protrusion is located at the intersection of the cross. For wafer 6, the single polyimide protrusion is $48\text{ }\mu\text{m}$ tall with a radius of $41.5\text{ }\mu\text{m}$ at the top and 47

Figure 3.1: An SEM of the single polyimide protrusion on wafer 6 after the experiments were completed. The protrusion is $48\text{ }\mu\text{m}$ tall with a radius of $41.5\text{ }\mu\text{m}$ at the top and $47\text{ }\mu\text{m}$ at the base. There are 22, $48.5\text{ }\mu\text{m} \times 48.5\text{ }\mu\text{m}$ square platinum microelectrodes arranged in a cross pattern around the protrusion. XBD 9507-03102.BIM

Figure 3.2: An SEM of the polyimide protrusion array on wafer 8 after the experiments were completed. The protrusions are $50\text{ }\mu\text{m}$ tall with a radius of $41.5\text{ }\mu\text{m}$ at the top and $47.5\text{ }\mu\text{m}$ at the base. XBD 9507-03491.BIM

μm at the base. For wafer 8, the protrusions in the array are $50\ \mu\text{m}$ tall with a radius of $41.5\ \mu\text{m}$ at the top and $47.5\ \mu\text{m}$ at the base, and the microelectrodes are arranged around the central protrusion in the array. The difference in radii is mainly due to a footer near the base of the protrusion (see Figure 3.1).

The different layers in the device can be described using Figure 3.3 as a guideline. The layers are split into three levels. The top level consists of $0.2\ \mu\text{m}$ of platinum on top of $0.2\ \mu\text{m}$ of titanium. The Ti/Pt bilayer is segmented into 22 microelectrodes, and a single cylindrical protrusion is drawn at the intersection of the cross formed by the microelectrodes. The middle level consists of a $1\ \mu\text{m}$ thick insulating layer of low-temperature oxide (LTO). Electrical connection between the aluminum lines and the platinum electrodes are made through openings in the LTO, where the openings are not shown for the buffer-electrode connections. The bottom level consists of $0.5\ \mu\text{m}$ thick aluminum lines on a thermally oxidized silicon wafer. The aluminum lines extend beyond the boundaries of the figure where the external connections are made. The aluminum lines can be seen through the Pt layer in Figure 3.1. The silicon wafer substrate is about $500\ \mu\text{m}$ thick. There is one layer that is not shown because it does not appear over the electrode region of the wafer. This is a hard-baked photoresist layer that is applied after all other fabrication is finished. This photoresist layer provides corrosion protection for the aluminum lines.

The platinum buffer electrode is superimposed on the aluminum metalization layer in the schematic in Figure 3.4. The aluminum lines are white on a grey background, and the buffer electrode is transparent but outlined in black. The aluminum lines near the center of the device are too small to be seen in Figure 3.4. Near the left and right of the schematic, the aluminum lines terminate at aluminum pads where the external connections are made to printed circuit boards. The lines to the microelectrodes are numbered 1 to 22 (the order in which they are sampled during the experiments), and the lines to the buffer electrode are labeled A to D. Lines 1 to 22 are $100\ \mu\text{m}$ wide near the external connection pads. Near the top and bottom of the schematic there are two white squares, labeled FCAM (standing for flow-cell alignment mark), that are located $1.374\ \text{cm}$ apart. These squares are used to

Figure 3.3: A schematic of the different layers in the device. The layers are split into 3 levels. The top level shows the Ti/Pt layer. The Ti/Pt layer consists of 22 Pt microelectrodes embedded within but electrically isolated from the large Pt electrode. The large Pt electrode is not shown in its entirety. The middle level shows the low-temperature oxide layer with 22 openings for the connections between the microelectrodes and the aluminum lines. The openings for the large electrode are not shown. The bottom level shows 22 aluminum lines on top of a thermally oxidized Si wafer (thickness not to scale).

Figure 3.4: A schematic showing platinum buffer electrode (transparent, but outlined in black) superimposed on the entire aluminum metalization layer (white lines on a grey background). The aluminum lines to the microelectrodes are numbered 1 to 22, and the aluminum lines to the buffer electrode are labeled A to D. The aluminum lines near the center of the device are too small to be seen. There are two white squares, labeled FCAM, located 1.374 cm apart near the top and bottom of the schematic that are used to align the flow cell to the microelectrodes.

align the flow cell to the microelectrode pattern. Finally, there is an arrow which is used to determine the wafer orientation. There are several other patterns in the schematic that serve no practical purpose.

The platinum buffer electrode, the vias through the oxide, and the aluminum metalization layer are superimposed in Figure 3.5. The vias for the external connection pads are two long rectangular openings. The vias for the platinum buffer electrode are four rectangles of two different sizes.

A close up of the aluminum lines near the center of the device is shown in Figure 3.6. In this region, the lines are $10\text{ }\mu\text{m}$ wide, and they terminate at $30\text{ }\mu\text{m}$ square pads numbered 1 to 22, where 1 to 11 are aligned in the flow direction and 12 to 22 are aligned transverse to the flow. The center-to-center distance is $50\text{ }\mu\text{m}$ between adjacent pads. The S-direction (*i.e.*, the sampling direction) and the AS-direction (*i.e.*, against the sampling direction) are also designated in Figure 3.6. These terms are used to describe the direction in which the electrolyte is traveling through the flow channel during a given measurement.

The white plus symbols (+) in Figure 3.6 designate possible locations for polyimide protrusions (some locations are not marked). One plus symbol is at the intersection of the microelectrode cross pattern. Microelectrodes 6 and 17 are the closest to this protrusion, with a center-to-center distance of $100\text{ }\mu\text{m}$. Microelectrodes 7 and 18 are the next closest, with a center-to-center distance of $125\text{ }\mu\text{m}$. By taking measurements in both the S- and AS-directions with this electrode arrangement, the local microelectrode current is obtained at $25\text{ }\mu\text{m}$ intervals between $100\text{ }\mu\text{m}$ and $350\text{ }\mu\text{m}$, both upstream and downstream of the protrusion.

The flow cell is superimposed on the aluminum lines and the buffer electrode in the schematic in Figure 3.7. The full length of the flow cell is not shown. The outer and inner walls of the flow cell are shown as black lines, and the o-ring used to seal the flow cell is shown as thick black lines. The outer walls are aligned to the flow-cell alignment marks, and the inner walls (0.3175 cm apart) cover part of the electrode, reducing the effective electrode width.

Figure 3.5: A schematic showing the superimposition of the entire aluminum metallization layer (the white lines against the grey background), the platinum buffer electrode (transparent, but outlined in black), and the via through the oxide (the solid black squares). The vias through the LTO for the outer aluminum pads are two long rectangular openings.

Figure 3.6: A schematic showing the small aluminum lines near the center of the device. The aluminum lines to the microelectrodes are numbered 1 to 22. The lines are numbered in the order in which the measurements are taken.

Figure 3.7: A schematic showing the flow cell superimposed on the aluminum metalization layer and the platinum buffer electrode.

Figure 3.8 shows the platinum microelectrodes in relation to the array of polyimide protrusions. The array has a square pitch oriented at 45° to the flow direction. The nearest neighbors are $318\text{ }\mu\text{m}$ apart (center-to-center distance), but the protrusions are $450\text{ }\mu\text{m}$ apart in the flow direction and the transverse direction. This array geometry was chosen because it is the closest packed regular array that could be placed around the microelectrode cross pattern. From the central protrusion, the array repeats 6 times in the upstream/downstream direction and 2.5 times in the transverse direction. Also, the edge of the central protrusion is about $28\text{ }\mu\text{m}$ from the ion-milled boundary of the closest microelectrode (assuming the central protrusion has a radius of $47\text{ }\mu\text{m}$ at its base). In hindsight, the distance between the microelectrodes and the protrusions could have been reduced (perhaps to $5\text{ }\mu\text{m}$).

Figure 3.9 shows a schematic of the flow cell in the vicinity of the buffer electrode (labeled as the working electrode). The flow cell has a square cross section with a width (W) of 0.3175 cm . A 2 cm long platinum counterelectrode is positioned on the wall opposite to the working electrode. A 0.5 mm diameter reference electrode port, which is located 1 cm upstream/downstream (the flow direction can be reversed) of the counterelectrode edge, is connected to a mercury/mercurous sulfate reference electrode located external to the cell. The reference electrode port was located far from the working electrode to avoid introducing disturbances in the flow. Finally, an (X,Y,Z) coordinate system is introduced in this figure, where capital letters are used to distinguish this coordinate system from the coordinate system defined in Figure 2.3. $X=0$ is the surface of the working electrode, $Z=0$ is the right flow-cell wall (for an observer looking in the flow direction), and $Y=0$ is the leading edge of the electrode. The origin of this coordinate system depends on the flow direction.

The two pictures in Figure 3.10 show the initial steps associated with loading a finished microelectrode device (or simply "a device") into the electrochemical cell. In the top picture, the device has a gold hue due to the photoresist layer, which serves as an additional protective layer for the aluminum lines against corrosive attack from the electrolyte. The device rests on a Plexiglas holder (1.9 cm thick with a $500\text{ }\mu\text{m}$ thick groove for the device to

Figure 3.8: A schematic showing the superimposition of the array of polyimide protrusions (dark circles), the platinum buffer electrode (transparent but outlined in black), the platinum microelectrodes (transparent but outlined in black), and the inner wall of the flow cell (heavy black lines).

Figure 3.9: A schematic showing the relative sizes of the working electrode and the counter electrode and the position of the reference electrode port. The flow channel is $0.3175 \text{ cm} \times 0.3175 \text{ cm}$ square in cross section.

rest in), and it is sandwiched between two other Plexiglas sheets (extender sheets—1.9 cm thick). These three Plexiglas pieces rest on a base sheet of Plexiglas (1.9 cm thick), which is held rigid by 4, $2.54 \text{ cm} \times 2.54 \text{ cm} \times 56 \text{ cm}$ aluminum bars. The tops of the device and the extender sheets are leveled using metal shims of $25.4 \mu\text{m}$ minimum thickness. After leveling is complete, the device is removed from the Plexiglas holder, the edges of the device that lie adjacent to the extender sheets are coated with a thin layer of silicone rubber, and the device is placed back on the Plexiglas holder. Next, the extender sheets are hand-tightened with a bolt against the device, lightly, to avoid bending the device. The extender sheets are then bolted to the base sheet near to the device using 4, 0.635 cm bolts. The excess silicon rubber is removed, and the remaining is allowed to cure overnight.

This procedure creates a surface flush to within $25.4 \mu\text{m}$ without cracks. One may be concerned about flow disturbances introduced at the boundary between the device and the extender sheets. However, this is not of concern for two reasons. One, the disturbance from device-extender sheet boundary is 2 cm from the working electrode, and, two, the

Figure 3.10: Loading a finished microelectrode device into the electrochemical cell. Top: The finished device ($5.258\text{ cm} \times 7.493\text{ cm}$) is placed on a piece of Plexiglas and sandwiched between two others so that the surfaces lie flush. Bottom: The flow cell is placed across the device, and the external connections are made to the microelectrodes and the buffer electrode using two pieces of a printed circuit board.

disturbance does not occur in the mass-transport boundary layer, where irregularities have the greatest effect on mass transport.

In the bottom picture in Figure 3.10, the flow cell is aligned to the device using the flow-cell alignment marks, and the flow cell is screwed onto the extender sheets using 20, 0.635 cm bolts spaced 5.08 cm apart (2.54 cm apart at the ends of the flow cell). There are threaded holes spaced every 2.54 cm in the extender sheets, but all of these are not needed. These bolts are sufficient to hold the flow cell flush against the extender sheets, but further clamping (described later) is required over the microelectrode device. Note that there are also threaded holes in the extender sheets oriented at a 45° angle with respect to the flow cell in the bottom picture. The original intention was to use the 45° orientation for the flow cell in addition to the usual orientation, but the microelectrode devices did not last long enough to try this.

Two printed circuit boards (cut from the board designed by Dees [44]) are used to make electrical contact to the aluminum pads on the microelectrode device. W series connectors (Fujipoly Inc., catalogue number WSL-082) are placed between the board and the aluminum pads. The connectors are different from the Zebra connectors used by Dees [44], Whitney [45], and Sutija [5], but they serve the same function. They consist of a strip of silicone rubber (1.6 mm × 0.3 mm × 100 mm) penetrated by individual, gold-plated metal wires, slightly greater than 0.3 mm in length. The rubber deforms when pressure is applied, ensuring a uniform, low-resistance connection of < 1 ohm. Two plug-in jacks connect the printed circuit board to wires, which are assembled into a cable and lead to a junction box (described later).

In Figure 3.11 (top), the flow cell is fully bolted down, and all of the wires are connected. An H-shaped clamp is used to press the flow cell onto the device. The counterelectrode connection is made by attaching an alligator clip to a screw that protrudes from the top of the flow cell. The reference electrode port terminates at a hose barb on top of the cell, and the hose barb is connected to a 1.27 cm OD polyethylene tube, which is sealed with a hose clamp to a mercury/mercurous sulfate reference electrode. Figure 3.11

Figure 3.11: Top: The microfabricated device is completely loaded into the experimental apparatus. Bottom: a bottom view of the flow cell after it is removed from the apparatus. The flow channel is $0.3175\text{ cm} \times 0.3175\text{ cm}$ square in cross section. The flow channel is difficult to see, but the o-ring is clearly visible. Compare to Figure 3.7, where the o-ring and flow-channel boundaries are shown schematically from a top view.

Figure 3.12: A schematic of the flow-cell loop. The direction of the flow is reversed through the flow channel by closing valves A and opening valves B. Valve C and the valves labeled VENT are used only for degassing the flow-cell loop and are normally kept closed.

(bottom) shows a bottom view of the flow cell. The counterelectrode, o-ring groove, and flow channel are visible. The flow channel extends for approximately 60 hydraulic diameters ($W=0.3175$ cm) to either side of the counterelectrode.

The final design for the flow loop is shown in the schematic in Figure 3.12. The thermometer probes next to the flow cell and the heat exchanger were not present for all experiments. When the thermometer probes were not present, the electrolyte temperature was monitored in the electrolyte reservoir. These differences in the flow-cell loop will be noted when the individual experiments are described. The flow-cell tubing was made of 1.27 cm OD polyethylene with 0.157 cm thick walls. The valves were made of polyvinyl

chloride, and the T-junctions and right-angle junctions were made of polyethylene.

The electrolyte was recycled through the loop using a centrifugal pump, and the flow rate was monitored using either a high- or a low-flow-rate rotameter. The low-flow-rate rotameter measured flow rates from 40 ml/min to 270 ml/min, corresponding to Reynolds numbers from about 200 to 1800, depending on the electrolyte temperature. The Reynolds number is defined by

$$\text{Re} = \frac{W u_b}{\nu} = \frac{Q}{\nu W}, \quad (3.1)$$

where ν is the kinematic viscosity, u_b is the average channel velocity, and Q the volumetric flow rate. The high-flow-rate rotameter measured flow rates from 300 ml/min to 1800 ml/min, corresponding to Reynolds numbers from about 2000 to 12000. A 20 liter polyethylene carboy held the electrolyte (4 liters), which was purged of oxygen with nitrogen gas for 1 hour before an experiment. A one-pass glass heat exchanger was connected to the flow-cell loop after the centrifugal pump. Two mercury thermometers, located on either side of the flow cell, were connected to the flow loop, by sealing the thermometers to one opening of a T-junction using a hose clamp. The other two ends of the T-junction were connected to the polyethylene tubing. During an experiment, the electrolyte temperature was controlled by adjusting the cooling-water flow rate directly at the faucet.

In Figure 3.12, the valve labeled C and the valves labeled VENT were used to remove trapped air while priming the flow loop, and they were closed during an experiment. The flow direction was reversed by closing valves A and opening valves B.

A schematic of the electronics is shown in Figure 3.13. The multiplexer, the current follower, the junction box, and the port for additional multiplexer inputs were assembled by Dees [44]. A Princeton 173 potentiostat with a 273 interface is used to control the electrode potential. The junction box is used to change the microelectrode wiring to access different channels in a 120-channel current follower (Scribner Associates, Inc.). The current follower produces a 1 V signal for every microamp of current, and it has an input impedance of 10 ohm. The microelectrode connections exit the current follower at a common output, which

Figure 3.13: A block diagram of the electronics for the experimental apparatus.

is attached to the working electrode connection of the potentiostat. The buffer electrode wiring is connected to a common bus bar in the junction box (shown as the dark line on the right side of the junction-box schematic), which is also connected to the working-electrode connection of the potentiostat.

The potential signal from the current follower is read by a computer-controlled 128-channel multiplexer (system 620/series 400 multiplexer by Neff Instrument Corporation), which contains a 10 Hz filter to eliminate nearly all high-frequency noise. All 22 channels are sampled in 17.6 ms (0.8 ms/microelectrode). The multiplexer also reads a potential that is proportional to the total electrode current and the potential of the working electrode through the additional multiplexer inputs. The readings from the multiplexer are stored on a 286 IBM clone computer. A single scan consists of sampling the 22 microelectrodes, the total current, and the applied potential. The time at which the scan is taken is recorded automatically. The rotameter reading, the electrolyte temperature, the flow direction are recorded manually in the computer.

3.3 Electrode reactions and limiting-current curves.

In this section, the electrode reaction and the limiting-current curves are described for our electrochemical cell. For a detailed discussion of the limiting-current technique, the reader is referred to a review article by Selman and Tobias [3].

A ferric/ferrous redox couple is used instead of a deposition reaction so that the electrode geometry would remain constant during the course of an experiment. The working electrode reaction is

and the counterelectrode reaction is the reverse reaction. The approximate electrolyte composition for each of the experiments was 0.05 M FeSO_4 , 0.05 M $\text{Fe}_2(\text{SO}_4)_3$, and 0.5 M H_2SO_4 . The exact concentrations are given in Table 3.1. According to Swift and But-

Table 3.1: Summary of experiments.

Experiment description	Experiment summary
no protrusion wafer 12	$[\text{Fe}_2(\text{SO}_4)_3] = 0.025 \text{ M}$ $[\text{FeSO}_4] = 0.050 \text{ M}$ $[\text{H}_2\text{SO}_4] \approx 0.5 \text{ M}$
single protrusion wafer 6	$[\text{Fe}_2(\text{SO}_4)_3] = 0.0255 \text{ M}$ $[\text{FeSO}_4] = 0.050 \text{ M}$ $[\text{H}_2\text{SO}_4] \approx 0.5 \text{ M}$ Protrusion height = $48 \mu\text{m}$ Radius at base of protrusion = $47 \mu\text{m}$ Radius at top of protrusion = $41.5 \mu\text{m}$
protrusion array wafer 8	$[\text{Fe}_2(\text{SO}_4)_3] = 0.025 \text{ M}$ $[\text{FeSO}_4] = 0.050 \text{ M}$ $[\text{H}_2\text{SO}_4] \approx 0.5 \text{ M}$ Protrusion height = $50 \mu\text{m}$ Radius at base of protrusion = $47.5 \mu\text{m}$ Radius at top of protrusion = $41.5 \mu\text{m}$

ler [46], the open-circuit potential (OCP) of reaction 3.2 in 1 M H_2SO_4 is 0.04 V *vs.* the saturated $\text{Hg}/\text{Hg}_2\text{SO}_4$ reference electrode.¹ The potential of the saturated $\text{Hg}/\text{Hg}_2\text{SO}_4$ reference electrode is 0.64 V *vs.* the normal hydrogen electrode (NHE). Hence, the equilibrium potential of reaction 3.2 is 0.68 V *vs.* the NHE.

Figure 3.14 shows limiting-current curves obtained in the flow cell for Reynolds numbers (*cf.*, equation 3.1) between 140 and 12600. The curves were obtained by scanning the potential in both the cathodic and anodic directions at 56 mV/s, except for the data for $\text{Re}=140$ which were obtained at 8 mV/s. A platinum electrode with the same dimensions as the buffer electrode was used, but it had no microelectrodes. The current is plotted against the total potential difference measured between the working electrode and a $\text{Hg}/\text{Hg}_2\text{SO}_4$

¹The concentration of sulfuric acid affects the open-circuit potential because the sulfate ions complex with the ferric ions to various degrees [47]. The standard equilibrium potential of reaction 3.2 is 0.78 V *vs.* the NHE.

Figure 3.14: Limiting-current curves for the ferric/ferrous redox couple in our flow cell apparatus at $Re = 140$ to 12600 . $\Delta\Phi_{\text{total}}$ is the difference between the working electrode potential and a mercury/mercurous sulfate reference electrode. The symbols represent data, and the lines are theoretical curves fit to the data. The parameters used in the fit are $\text{OCP} = 0.015 \text{ V}$, $i_o = 0.015 \text{ A}/\text{cm}^2$, and $\rho = 4.3 \text{ ohm}\cdot\text{cm}$.

reference electrode, $\Delta\Phi_{\text{total}}$. $\Delta\Phi_{\text{total}}$ is given by

$$\begin{aligned}\Delta\Phi_{\text{total}} &= \Phi_{\text{working}} - \Phi_{\text{reference}} \\ &= \text{OCP} + \Delta\Phi_{\text{ohmic}} + \eta\end{aligned}\tag{3.3}$$

where $\Delta\Phi_{\text{ohmic}}$ is the ohmic drop and η includes both concentration and charge-transfer overpotential.

In Figure 3.14, the symbols represent the data, the dashed lines represent the theoretical curves without ohmic drop, and solid lines represent the theoretical curves with ohmic drop. The equations used to calculate the theoretical curves appear in Appendix C. The model is very simple because mass transport and ohmic drop across the electrode are assumed to be uniform and because hydrogen evolution is not included. The solution resistance is estimated using a resistivity of 4.287 ohm-cm (the interpolated value for 5 wt% sulfuric acid (~ 0.5 M H_2SO_4) reported by Lobo [48]) and the distance between the working electrode and the counterelectrode (0.3175 cm). The other parameters required for the theoretical calculations are the OCP, the ratio of the exchange current density to the limiting current density (i_0/i_l), and the apparent anodic and cathodic transfer coefficients (α_a and α_c). The OCP was set to 0.015 V instead of 0.04 V to account for the calibration of the $\text{Hg}/\text{Hg}_2\text{SO}_4$ reference electrode. An exchange current density of 0.015 A/cm² and transfer coefficients of $\alpha_a = \alpha_c = 0.5$ were used, in rough agreement with literature values [49] for our electrolyte concentration.

Accounting for the calibration of the reference electrode, hydrogen evolution should occur at approximately -0.665 V, but hydrogen evolution actually begins between -0.72 V to -0.77 V for each of the limiting-current curves. Slightly more negative potentials are required at higher Reynolds numbers because the limiting current increases leading to increased ohmic drop. For each of our subsequent mass-transfer experiments, the potential, $\Delta\Phi_{\text{total}}$, was set to -0.6 V *vs.* the reference electrode. At this potential, the current appears to be mass-transfer limited for the entire Reynolds number range, and hydrogen is not evolved.

Since the limiting current increases with Reynolds number, the limiting-current

curves become obscured by ohmic drop. That is, the limiting-current curves become shorter and less well defined. This is because the ohmic drop at the electrode edges is lower than the ohmic drop to the rest of the electrode. As a result, a higher $\Delta\Phi_{\text{total}}$ is required to attain limiting currents over the entire electrode, but the $\Delta\Phi_{\text{total}}$ at which hydrogen is evolved near to the electrode edges will be relatively unaffected. Our model is not sophisticated enough to capture these effects. To see a detailed model, the reader is referred to White and Newman [50]. They studied the effect of nonuniform potential distribution and the effect of secondary reactions on the shape of the limiting current curves for copper deposition to a rotating disk electrode from an electrolyte containing copper sulfate and sulfuric acid.

For a segmented microelectrode, the potential of each microelectrode and the buffer electrode is slightly different because of ohmic drop across the aluminum lines. A worst-case scenario is examined to show that this is not a problem for a typical device. The resistance of a typical aluminum line to a microelectrode is about 100 ohms. The resistances of the four aluminum lines to the buffer electrode are smaller because the lines are wider, and their total resistance in parallel is about 0.5 ohms. If the highest current density to the buffer electrode and the microelectrodes electrodes is about 83 mA/cm², then the worst-case ohmic drop for the buffer electrode (electrode area 0.16 cm²) is about 6.5 mV, and the worst-case ohmic drop for the microelectrodes (electrode area 2.35×10^{-5} cm²) is about 0.2 mV. In view of the size of the potential window in which the current is limiting, a 6.3 mV potential difference between the buffer electrode and the microelectrodes is tolerable.

3.4 Mass transport in the absence of protrusions

3.4.1 The general form of the Lvque solution for both turbulent and laminar flow

In this section, the theoretical background current distribution to the working electrode in our square flow cell is predicted for turbulent and laminar flow. The background current distribution is defined as the current distribution to the working electrode in the

absence of protrusions. In Chapter 4, the background current is used to normalize the data or for comparison to the data. For turbulent flow, the background current is only needed in the flow direction since we were unable to obtain current distributions in the transverse direction (see discussion in Section 3.5).

To simplify the equations of convective diffusion for the laminar flow case, several simplifying assumptions are made:

1. Dilute solution theory applies.
2. The density of the electrolyte is constant.
3. The diffusivity of ferric ions, D_a , is constant.
4. The flow is fully developed.
5. Migration effects are ignored.

With these assumptions, the convective diffusion equation for species A (the ferric ions) simplifies to

$$u_y \frac{\partial C_a}{\partial Y} = D_a \left(\frac{\partial^2 C_a}{\partial X^2} + \frac{\partial^2 C_a}{\partial Y^2} + \frac{\partial^2 C_a}{\partial Z^2} \right) \quad (3.4)$$

where C_a is the concentration of ferric ions, the spatial variables X , Y , Z correspond to the coordinate system in Figure 3.9, and the quantities including u_x and u_z were omitted because these terms are identically equal to zero.

In regard to assumption 2, it is noted that density changes for redox reactions are generally less than for deposition reactions. In regard to assumption 4, the hydraulic entry length, L_h , for fully developed flow is estimated. For circular pipes, L_h is given by

$$L_h/D \approx 0.59 + 0.055 \text{ Re} , \quad (3.5)$$

where D is the diameter of the pipe [51]. Replacing D by the hydraulic diameter W for a square duct, the available entry length in our flow cell ($\sim 60W$) is less than L_h up to about $\text{Re}=1000$. However, this criterion may be too strict for our purposes. As will be

shown, only the shear rate at the wall needs to be fully developed. Therefore, the flow will always be assumed to be fully developed. In regard to assumption 5, sulfuric acid was added in ten-fold excess of the ferric and ferrous ions to reduced migration effects. Whether migration increases or decreases the flux of ferric ions to the cathode is unclear because the ferric species exists as a mixture of positive and negative complexes in solution [47] ($\text{Fe}(\text{SO}_4)^+$, $\text{Fe}(\text{SO}_4)_2^{2-}$, and $\text{Fe}(\text{SO}_4)_3^{3-}$). However, the effect is probably small based on the effect of migration in the ferrocyanide/ferricyanide system in the presence of ten-fold excess potassium hydroxide. Newman [52] modeled this system and found that migration altered the mass flux by about 1% relative to diffusion only.

To simplify equation 3.4 further, the following additional assumptions are made

6. The mass-transfer boundary layer is thin compared to the dimensions of the flow cell.
7. Diffusion in the flow direction (the Y direction) is small compared to convection in the flow direction.
8. Diffusion in the transverse direction (the Z direction) is small compared to convection in the flow direction.

Equation 3.6 now simplifies to

$$\beta X \frac{\partial C_a}{\partial Y} = D_a \frac{\partial^2 C_a}{\partial Y^2} \quad (3.6)$$

where the Y -component of velocity is approximated by βX and β is the shear rate at the wall. This approximation for the velocity is justified by assumption 6. The simplifications leading to equation 3.6 were first recognized by Lvque [53], and the solution of equation 3.6 is commonly referred to as the Lvque solution.

Assumption 6 is valid only in the mass-transfer entrance region, L_e . For laminar flow through an annulus, Ross and Wragg [54] estimate that the entry length is approximately

$$L_e = 0.005 \text{ Re Sc } d_h \quad (3.7)$$

where d_h is the hydraulic diameter. Replacing d_h with W , estimating the Schmidt number of the electrolyte to be 1600, and using $Re=100$ as the minimum Reynolds number, L_e is estimated to be $800W$. Since length of the buffer electrode is only $1.57W$, assumption 6 is valid in laminar flow.

Assumptions 7 and 8 eliminate the diffusion terms in the flow and transverse directions, respectively. Diffusion in the flow direction is eliminated because the Péclet number

$$Pe = \frac{Wu_b}{D_a} \quad (3.8)$$

is approximately 170,000 at $Re=100$. This implies that diffusion in the flow direction is much smaller than convection in the flow direction. Similarly, diffusion in the transverse direction is much smaller than convection in the flow direction, except at small distances from the side walls where the velocity goes to zero.

The boundary conditions for equation 3.6 are

$$C_a = \bar{C}_a \quad \text{as} \quad X \rightarrow \infty \quad (3.9)$$

$$C_a = \bar{C}_a \quad \text{at} \quad Y = 0$$

$$C_a = 0 \quad \text{at} \quad X = 0$$

where $\bar{C}_a$ is the bulk concentration in solution. The solution procedure for the concentration profile is outlined by Newman [52, pages 348-9] and Bird, Stewart, and Lightfoot [55, pages 551-2, problem 17.J]. The solution is

$$C_a = \frac{\bar{C}_a}{\Gamma(\frac{4}{3})} \int_0^\eta e^{-\xi^3} d\xi \quad (3.10)$$

where

$$\eta = X \left(\frac{\beta}{9D_a Y} \right)^{\frac{1}{3}} \quad (3.11)$$

and Γ is the gamma function. The local flux to the electrode is given by

$$N_a = -D_a \frac{dC_a}{dX} \Big|_{X=0} = -D_a \frac{\bar{C}_a}{\Gamma(\frac{4}{3})} \left(\frac{\beta}{9D_a Y} \right)^{\frac{1}{3}} \quad (3.12)$$

The local flux is related to the local current density, i_n , by Faraday's law [52, page 336]

$$i = -\frac{nF}{s_a} N_a \quad (3.13)$$

where s_a is the stoichiometric coefficient for species a (negative for cathodic reactants) and n is the number of electrons participating in the reaction. Substituting 3.13 into 3.12 gives

$$i = \frac{nFD_a\bar{C}_a}{s_a\Gamma(\frac{4}{3})} \left(\frac{\beta}{9D_aY} \right)^{\frac{1}{3}} \quad (3.14)$$

For reaction 3.2, $s_a = -1$ and $n = 1$.

Equation 3.14 predicts a nonuniform current distribution across the electrode because β is expected to be nonuniform across the channel width. Since β is zero at the side walls, equation 3.14 predicts that the current density is zero at these points. In actuality, the current is not zero because assumptions 7 and 8 break down at the side walls. Equations for β are given in the next section.

Equation 3.6 also applies for turbulent flow, but further assumptions are needed:

9. The eddy diffusivity is negligible.

10. Secondary flows are negligible.

Linton and Sherwood [56] were the first to apply equation 3.6 to turbulent flows. For turbulent flow, it is implicitly implied that equation 3.6 is time averaged.

Assumptions 1 to 8 still apply, but the hydraulic entry length criterion is different for turbulent flow. Typically, 40 hydraulic diameters are more than sufficient for turbulent flow to become fully developed. Our flow cell has 60 hydraulic diameters of entry length, which is more than sufficient.

Assumption 9 is valid only in the mass-transfer entry region for turbulent flow, which is much shorter than the mass-transfer entry region for laminar flow. From the results of Shaw *et al.*, the mass-transport entry region is ~ 2 hydraulic diameters at $Re=20000$ and ~ 3 hydraulic diameters at $Re=5000$. Since the buffer electrode is $1.57W$, assumption 9 is reasonable. Assumption 10 is required because low-magnitude secondary flows, transverse

to the bulk flow, are induced by the turbulence. The average magnitude of the secondary velocity is about 2 to 3% of the average downstream velocity [57]. The experiments by Goldstein *et al.* [58] suggest that the secondary flow enhances mass transfer near the corners of a square duct, but the flow does not significantly affect mass transfer elsewhere. Since we are not interested in mass transfer near the corners of the duct, the secondary flows are ignored.

3.4.2 The Lvque solution for laminar flow in a square duct

For laminar flow in a square duct, the velocity profile is given by Happel and Brenner [59, page 38]

$$u_y = -\frac{4Q}{\pi W^4} X(X - W) + \sum_{m=1}^{\infty} \sin \frac{m\pi X}{W} \left[A_m \cosh \frac{m\pi Z}{W} + B_m \sinh \frac{m\pi Z}{W} \right], \quad (3.15)$$

where

$$A_m = \frac{16Q}{m^3 \pi^4 W^2} (\cos(m\pi) - 1), \quad (3.16)$$

$$B_m = -\frac{A_m (\cosh(m\pi) - 1)}{\sinh(m\pi)}, \quad (3.17)$$

Q is the volumetric flow rate, and W is the channel width. The velocity is zero on the channel walls ($X = 0$, $X = L$, $Z = 0$, $Z = L$). Taking the derivative of equation 3.15 with respect to X gives

$$\begin{aligned} \beta &= \left. \frac{du_y}{dX} \right|_{X=0} \\ &= \frac{4Q}{\pi W^3} + \sum_{m=1}^{\infty} \frac{m\pi}{W} \left[A_m \cosh \frac{m\pi Z}{W} + B_m \sinh \frac{m\pi Z}{W} \right] \end{aligned} \quad (3.18)$$

for the shear rate at the wall. Equation 3.18 gives an estimate for β at a given transverse position Z from the measured volumetric flow rate Q .

Equation 3.14 and Equation 3.18 can be used to calculate the average current density to an electrode in a square channel. Averaging over the channel width W gives

$$\langle i \rangle_W = 1.88 \frac{nFD_a \bar{C}_a}{s_a \Gamma(\frac{4}{3})} \left(\frac{Q}{9D_a Y W^3} \right)^{\frac{1}{3}}, \quad (3.19)$$

and averaging over both the channel width W and the electrode length L gives

$$\langle i \rangle_{WL} = 2.823 \frac{nFD_a \bar{C}_a}{s_a \Gamma(\frac{4}{3})} \left(\frac{Q}{9D_a LW^3} \right)^{\frac{1}{3}}. \quad (3.20)$$

The subscript W or WL indicates that the quantity in brackets was averaged over the channel width or over both the channel width and the channel length. Dividing equation 3.14 by equation 3.19 yields

$$\frac{i}{\langle i \rangle_W} = 0.532 \left(\frac{\beta W^3}{Q} \right)^{\frac{1}{3}}, \quad (3.21)$$

which does not depend on the downstream position Y . This means that the local current distribution across the electrode will appear the same for any downstream position if the current is normalized by $\langle i \rangle_W$.

The ratio $i/\langle i \rangle_W$ is plotted against the dimensionless transverse position across the flow cell in Figure 3.15. The solid line is from equation 3.21, and the dashed lines are the numerical solutions of equation 3.4 calculated using FIDAP for $Re=205$ and $Sc=2500$ and at $Y/L=0.21$ and 0.92 . The numerical results at both downstream positions are in general agreement with equation 3.21, justifying assumptions 6, 7, and 8 away from the side walls. A greater mesh density would be needed to determine where the Lvque solution breaks down near the side walls, but it is only important that the solution is valid across the central 22% of the flow cell, the distance spanned by the microelectrodes. Note that the numerical results are plotted in a stair-step pattern (the asymmetry is possibly due to numerical inaccuracies) because the flux is averaged over each element by the program. Furthermore, it is noted that the average current densities calculated by FIDAP and the Lvque solution agree to within 1%, justifying equations 3.19 and 3.20.

A surface projection of the mesh that was used with FIDAP is shown in Figure 3.16. The entire 0.5 cm length by 0.3175 cm width of the electrode was meshed. However, only a 0.05 cm vertical distance from the electrode was discretized because the mass-transport boundary-layer thickness is only on the order of 0.01 cm thick. Equation 3.15 was used to assign the local velocities before the convective diffusion equation was solved.

Figure 3.15: The local current density for laminar flow as a function of transverse position across an electrode in a square flow cell when no protrusions are present on the electrode surface. The FIDAP results form a stair-step pattern because the local current is averaged over an element width.

Figure 3.16: Mesh used for solving the mass-transport distribution in a square flow channel. The mesh extends only 0.05 cm from the electrode for a 0.3175-cm wide flow cell.

Finally, equation 3.20 is written in terms of dimensionless quantities:

$$\langle \text{Sh} \rangle_{WL} = 1.520 \text{Re}^{1/3} \text{Sc}^{1/3} (W/L)^{1/3}, \quad (3.22)$$

where the average Sherwood number is given by

$$\langle \text{Sh} \rangle_{WL} = \frac{\langle i \rangle_{WL} s_a W}{n F \bar{C}_a D_a} \quad (3.23)$$

and where $\Gamma(\frac{4}{3})$ was replaced with 0.89298. In Appendix D, $\langle \text{Sh} \rangle_{WL} / \text{Sc}^{1/3}$ is plotted against Re for the experimentally measured current to the entire electrode.

3.4.3 The Lvque solution for turbulent flows

The universal velocity profile [60, page 166] is used to predict the velocity distribution. Hartnett *et al.* showed that the universal velocity profile provides a good approximation for the velocities in a rectangular duct [61], except near the corners where the secondary flows have the greatest influence. Near the wall, the universal velocity profile is linear and is given by

$$u_y^+ = X^+, \quad (3.24)$$

where $u_y^+ = u_y / u^*$ and $X^+ = Xu^* / \nu$ are dimensionless quantities, and $u^* = \sqrt{\tau_w / \rho}$ is the friction velocity. The friction velocity is related to a friction factor, f , by $f = 2(u^*)^2 / u_b$. Rearranging equation 3.24 to dimensional form gives

$$u_y = \left(f \text{Re} \frac{Q}{2W^3} \right) X. \quad (3.25)$$

The friction factor can be related to the Reynolds number by the empirical equation of Blasius [60, page 168]

$$f = 0.079 \text{Re}^{-0.25}. \quad (3.26)$$

Taking the derivative of equation 3.25 with respect to X and substituting equation 3.26 for the friction factor gives

$$\begin{aligned} \beta &= 0.0395 \text{Re}^{0.75} \frac{Q}{W^3} \\ &= 0.0395 \text{Re}^{1.75} \frac{\nu}{W^2}. \end{aligned} \quad (3.27)$$

β can then be estimated if the flow rate and (unlike laminar flows) the kinematic viscosity are known. In the transition between laminar and turbulent flow ($2100 < \text{Re} < 3000$) equation 3.26 overpredicts the value for the friction factor. As a result, the value for the shear rate will also be high in this Reynolds-number range. Equation 3.27 does not predict a Z dependence for the shear rate. This means that equation 3.27 in conjunction with equation 3.14 corresponds to a constant mass-transfer distribution across the square flow channel. In addition to the work of Hartnett *et al.* [61] mentioned above, this result is supported by the work of Goldstein *et al.* [58]. They found that the local sublimation rate of naphthalene into a turbulent air stream was relatively constant across the wall of a square duct except near the corners, where enhanced mass transport was observed. Since we require the background current only along the centerline of our electrode half way between the side walls, equation 3.27 in conjunction with equation 3.14 is sufficient for our needs.

Substituting equation 3.27 into equation 3.14 and averaging over the electrode width and length give

$$\langle \text{Sh} \rangle_{WL} = 0.276 \text{Re}^{0.58} \text{Sc}^{1/3} W/L^{1/3}, \quad (3.28)$$

where $\text{Re}^{0.58}$ is approximately equal to $(\text{Re}^{1.75})^{(1/3)}$. The exponent on the Reynolds number is the same exponent that Shaw *et al.* [62] predicted for short electrodes in turbulent flow. As for the laminar flow case, $\langle \text{Sh} \rangle_{WL}/\text{Sc}^{1/3}$ is plotted against Re in Appendix D for the experimentally measured current to the entire electrode for the turbulent flow case, and the results are compared to the expected values calculated using equation 3.28. When the electrode extends beyond the mass-transfer entry region, the exponent on the Reynolds number increases until the exponent corresponding to fully developed turbulent flow is achieved. The upper limit of the exponent is not as certain as the lower limit, but an estimated value of 0.8 is obtained from the Chilton-Colburn analogy [63, page 70]). Whatever the upper limit, the exponent determined from our $\langle \text{Sh} \rangle_{WL}/\text{Sc}^{1/3}$ vs. Re plots should be slightly high if the exponent does not agree with the 0.58 value exactly.

3.4.4 Experimental determination of the background current

To show that the Lvque solution actual applies to our system, current distributions were measured using segmented microelectrodes with no protrusions. The measurements were also used to determine the diffusivity of ferric ions in our electrolyte. The experiments were done at flow-cell Reynolds numbers between 240 and 10600 using wafer 12.

First, an average diffusivity was calculated from the laminar flow results. To do this, equation 3.14 was rearranged to give

$$D_a = \left(\frac{i s_a \Gamma(\frac{4}{3})}{n F C_a} \right)^{3/2} \left(\frac{9Y}{\beta} \right)^{1/2} \quad (3.29)$$

From equation 3.29, a value for the diffusivity can be calculated using the current density measured at a single microelectrode, i ; the downstream position of the microelectrode, Y ; and the value for the shear rate, β , which is estimated using equation 3.18. The average diffusivity from the laminar-flow measurements was $4.590 \times 10^{-6} \text{ cm}^2/\text{s}$ at 25.6°C . This compares favorably with the value of $4.351 \times 10^{-6} \text{ cm}^2/\text{s}$ reported by Whitney [45, pages 130, 137, 141] for 0.0484 to 0.110 M $\text{Fe}_2(\text{SO}_4)_3$ in 0.5 to 1.0 M H_2SO_4 at room temperature.

The current distributions in the flow direction and the transverse direction are shown in Figures 3.17 and 3.18, respectively, for $\text{Re}=240, 800, \text{ and } 1400$. To reduce the number of plots, the current density was normalized by $\langle i \rangle_{y=-350 \mu\text{m}}$, the the average current density at the (Y,Z) position corresponding to microelectrode 1 (*cf.*, Figure 3.6) assuming that the electrolyte is flowing in the S-direction. This average current was calculated by substituting $D_a = 4.590 \times 10^{-6} \text{ cm}^2/\text{s}$, $Y = 0.25 \text{ cm} - 0.035 \text{ cm} = 0.215 \text{ cm}$, and the shear rate β for the individual measurements into equation 3.14. The abscissas in Figures 3.17 and 3.17 are the downstream and transverse distances y and z , which are related to Y and Z by $Y = 0.25 \text{ cm} + y$ and $Z = 0.15875 \text{ cm} + z$, where $(y,z)=(0,0)$ corresponds to the intersection of the microelectrode cross pattern, 0.25 cm is half the electrode length in the flow direction, and 0.15875 cm is half the channel width. The solid lines are the theoretical current densities calculated using equation 3.14, equation 3.18, and the average

Figure 3.17: The local microelectrode current in the direction of flow without protrusions for $Re=240$, 800, and 1400 (wafer 12). The current is normalized by the average current at $y=-350 \mu m$. The filled data symbols were taken with the electrolyte flowing in the AS-direction, and the unfilled data symbols were taken with the electrolyte flowing in the S-direction. Each datum symbol at $Re=240$ and 800 represents a single measurement, and each datum symbol at $Re=1400$ is an average of 10 measurements.

Figure 3.18: The local microelectrode current in the transverse direction without protrusions for $Re=240$, 800, and 1400 (wafer 12). The current is normalized by the average current at $y=-350 \mu\text{m}$. The filled data symbols were taken with the electrolyte flowing in the AS-direction, and the unfilled data symbols were taken with the electrolyte flowing in the S-direction. Each datum symbol at $Re=240$ and 800 represents a single measurement, and each datum symbol at $Re=1400$ is an average of 10 measurements. Microelectrode 15 is partially inactive.

diffusivity. Curiously, the data points collected with the electrolyte flowing in the AS-direction tend to lie above the theoretical curve whereas the data points collected with the electrolyte flowing in the S-direction tend to lie below the theoretical curve. This tendency is accentuated with increasing Reynolds number. In Figure 3.17, for example, the AS-direction data lie 0.5%, 1.5%, and 2% above the S-direction data for $Re=240$, 800, and 1400, respectively. This systematic difference is possibly results from a small amount of asymmetry in the flow-cell apparatus.

For the flow direction, if the theoretical curve in Figure 3.17 were shifted to fit the S-direction data for any single scan, the data would deviate from the curve in a characteristic manner that would be nearly identical for every scan in this direction. This characteristic deviation is due to artifacts in the measurement device because it is not reproducible when the flow direction is reversed. Aside from these small deviations, the gross features of the measured current distributions are the same in both flow directions, which raises confidence in the experimental results. For example, the measured dimensionless current density decreases by roughly 9% over the distance spanned by the microelectrodes in both flow directions. This decrease is also in agreement with the theoretical current distribution.

For the transverse direction, the scatter in the data in Figure 3.18 is larger than the 1% variation in the theoretical background current density over the distance spanned by the microelectrodes. Also, as can be seen in the bottom graph with the reduced scale, microelectrode 15 is partially inactive. The microelectrode becomes more inactive with increasing Reynolds number relative to the properly functioning microelectrodes. This indicates that the measurements are less susceptible to errors at lower current densities. The current to the microelectrodes immediately adjacent to microelectrode 15 appear to be slightly enhanced, but the current to the microelectrodes that lie farther away do not appear to be affected.

Average diffusivities for turbulent flow are calculated by the same procedure used for laminar flow. However, the shear rate at the wall cannot be estimated with as much confidence as it was for laminar flow. The diffusivities calculated at $Re=2920$, 7900, and

10550, reported in Table 3.2, are all lower than the laminar-flow diffusivity calculated for $Re=240$ to 1400. This probably indicates that the shear rate predicted by equation 3.27 is

Table 3.2: Diffusivities calculated from the laminar- and turbulent-flow experiments with the assumption that the Lvque solution is valid.

Re	D_a (cm^2/s)	Temperature ($^\circ\text{C}$)
240 to 1400	4.590 ± 0.058	25.61 ± 0.14
2920	3.875 ± 0.203	25.81 ± 0.04
7900	4.197 ± 0.129	26.35 ± 0.49
10600	4.069 ± 0.149	25.74 ± 0.05

slightly higher than the actual value. A high shear rate gives a low value for the diffusivity from equation 3.29. The deviation is greatest at $Re=2920$, which is not surprising because $Re=2920$ is close to the laminar-turbulent transition where the accuracy of equation 3.27 is relatively low. Nevertheless, it appears that the Lvque solution gives a good order-of-magnitude estimate for the diffusivity even in turbulent flow.

The current distribution in the flow direction is shown in Figure 3.19 for $Re=2900$, 7900, and 10600. Each datum symbol is an average of 100 measurements. The diffusivities calculated at the individual Reynolds numbers were used to determine the theoretical solid lines. As for the laminar-flow results, the data collected with the electrolyte flowing in the AS-direction lie above the data collected with the electrolyte flowing in the S-direction. This is particularly noticeable at $Re=2900$. At $Re=2900$, the measured microelectrode current appears to decrease with downstream distance at the same rate as the theoretical curve. At $Re=7900$, however, the measured current appears to decrease at a slightly slower rate than the theoretical curve, probably because the transition to fully developed mass transfer has begun. The entrance length required to attain fully developed turbulent mass transport decreases with increasing Reynolds number because the eddy diffusivity increases. Wasan *et al.* [64] numerically modeled the transition region. At $Re=10600$ the measured microelectrode current still appears to decrease with downstream distance, but the electrode was beginning to fail at this point (after 70 minutes of measurements plus 1 hour of exposure

Figure 3.19: The local microelectrode current in the direction of flow without protrusions for $\text{Re}=2900$, 7900 , and 10600 (wafer 12). The filled data symbols were taken with the electrolyte flowing in the AS-direction, and the unfilled data symbols were taken with the electrolyte flowing in the S-direction.

to electrolyte while degassing the flow loop) as is noticeable by the artifacts in the data,² and it is difficult to determine the actual state of the transition.

The turbulent mass-transport distributions are not shown in the transverse direction. Although the data were collected by averaging 100 measurements at a time, reliable current distributions could not be obtained in the transverse direction. The reason for this is related to the scale of the turbulence, the topic of the next section.

3.5 Length scales, time scales, and current fluctuations in turbulent flow

In turbulent flow, it was significantly easier to obtain current distributions in the direction of flow than in the transverse direction. This was because the apparent current distribution in the direction of flow from a single scan appeared very similar to the time-averaged current distribution. In contrast, the apparent current distribution in the transverse direction from a single scan bore little to no resemblance to the time-averaged current distribution. As a result, significantly fewer scans were required to converge upon the final time-averaged current distribution in the direction of flow than in the transverse direction. Since the devices degraded at accelerated rates from the relatively high current densities in turbulent flow, it was deemed prudent to take a few scans quickly to obtain a current distribution in the direction of flow and to disregard the current distribution in the transverse direction.

Turbulent flow can be characterized by length scales, time scales, and turbulence intensity. Below, these quantities are determined adjacent to the electrode from our measurements or from literature values. From these quantities, it is determined whether or not it is surprising that the current distributions in the flow direction are correlated and that the current distributions in the transverse direction are not correlated. The results of this

²The microelectrodes, in general, tended to degrade more quickly while measuring higher current densities. However, the rate of degradation varied from device to device. The device with the protrusion array lasted the longest—about 300 minutes total exposure time.

analysis give us better understanding of the turbulent flows that were studied, but they are not needed to justify the results in Chapter 4.

Length and time scales adjacent to the electrode are considered first. The length scale can be thought of as the size of a eddy, and the time scale can be thought of as the lifetime of a eddy. To quantify these scales, a correlation coefficient, R_λ , is introduced, which is defined as

$$R_\lambda = \frac{\overline{I'(\lambda_0) I'(\lambda_0 + \lambda)}}{\sqrt{(\overline{I'(\lambda_0)})^2} \sqrt{(\overline{I'(\lambda_0 + \lambda)})^2}}, \quad (3.30)$$

where λ is replaced by y for correlations in the flow direction, by z for correlations in the transverse direction, and by t for correlations in time. Similarly, λ_0 represents either a reference time or a reference position. I' is the instantaneous deviation from the average current, and the overbar indicates that the quantity is averaged over time (or over $\lambda_0 = t_0$ for correlations in time). The correlation coefficient is unity when $\lambda = 0$. The correlation coefficients can be written as functions of both space and time simultaneously (see Kreplin and Eckelmann [65]), but this is not done here to keep the analysis relatively simple.

A length scale is defined in terms of the correlation coefficient to be

$$\Lambda_\lambda = \int_0^\infty R_\lambda d\lambda. \quad (3.31)$$

A time scale could be defined similarly, but values for a time scale defined in this manner were not found in the literature. However, since correlation coefficients as a function of time were found, the time scale, Λ_t , is defined to be the time corresponding to $R_t = 0.5$.

At this point, it is convenient to introduce dimensionless variables. For the length and time scales, Λ_λ , we define the variables $\Lambda_y^+ = u^* \Lambda_y / \nu$, $\Lambda_z^+ = u^* \Lambda_z / \nu$, and $\Lambda_t^+ = (u^*)^2 \Lambda_t / \nu$ where $u^* = \sqrt{\tau_w / \rho}$, u^* is the friction velocity, and τ_w is the shear stress at the wall. For time, we introduce the variable $t^+ = (u^*)^2 t / \nu$. The dimensionless length and time scales tend to vary less with Reynolds number than the dimensional length and time scales, and Λ_z^+ tends to vary less than Λ_y^+ or Λ_t^+ .

The time scale was obtained from current fluctuations to a single microelectrode

on a device with no protrusions. The fluctuations are shown in Figure 3.20 for a 4.5 s period and in Figure 3.21 for a 100 ms period, and the Reynolds number range is between 850 and 12200. The electrolyte composition was the same as the no-protrusion case listed in Table 3.1. The measurements were taken by connecting a high-speed digital oscilloscope directly to the current follower output and setting the sampling rate on the oscilloscope to 0.5 ms/point. The data at $Re=850$ are free of turbulent fluctuations. The ripples in the data are from noise, not turbulence because the ripples are periodic, not random (not apparent from figures). This noise is normally eliminated by the 10 Hz filter in the multiplexer. A slight disturbance, not attributable to noise, is first observed at Re of 1540. The fluctuations then become very noticeable at Re of 1990 and 2390.

The correlation coefficients, R_t , corresponding to the data in Figures 3.20 and 3.21 are plotted in Figure 3.22 for $Re=5000$, 9100, and 12200. In the top graph, the correlation coefficient is plotted against time, and, in the bottom graph, the correlation coefficient is plotted against dimensionless time. The correlation coefficient varies less with Reynolds number for the dimensionless time scale. The Λ_t and Λ_t^+ values corresponding to $R_t=0.5$ are given in a table at the bottom of the figure. The dimensional time scales, Λ_t , are 22.5 ms, 11.5 ms, and, 5.5 ms at $Re=5000$, 9100, and 12200. The dimensionless time scales, Λ_t^+ , varied between 207 and 302 (not monotonically) between $Re=5000$ and 12200. For simplicity, Λ_t^+ is estimated to be 250 over this Reynolds number range. In contrast, from the data of Hanratty [66], Λ_t^+ is estimated to be about 50 at $Re=62000$, and, from the data of Kreplin and Eckelmann [65], Λ_t^+ is estimated to be 20 at $Re=7700$. Our value for the time scale is about 5 to 10 times higher than the literature values. Possibly, this is because our time scale was measured using a microelectrode that was embedded within a larger active electrode. Usually, when turbulent fluctuations in the viscous sublayer are studied, isolated microelectrodes or heated probes are used to minimize the thickness of the mass transport or thermal-boundary-layer thicknesses and to improve the response time (see Reiss and Hanratty [67]).

Since data for the length scales were not obtained in this study, we turn to the

Figure 3.20: The unfiltered current density to a single microelectrode electrode (0.5 ms/point) over a 4.5 s period and for $Re=850$ to 12200.

Figure 3.21: The unfiltered current density to a single microelectrode electrode (0.5 ms/point) over a 0.1 s period and for $Re=850$ to 12200.

Re	Λ_t (ms)	Λ_t^+
5000	22.5	207
9100	11.5	302
12200	5.5	243

Figure 3.22: The correlation coefficient, R_t , for turbulent fluctuations adjacent to the electrode. R_t is plotted against time (top graph) and dimensionless time (bottom graph) for Reynolds numbers of 4970, 9050, and 12200. The dimensional time scale Λ_t and the dimensionless time scale Λ_t^+ corresponding to $R_t = 0.5$ are given in a table underneath the graphs.

Figure 3.23: Turbulence intensity adjacent to the electrode as a function of Reynolds number.

literature. Mitchell and Hanratty [68] found $\Lambda_z^+ \cong 11$ for Reynolds numbers between 7500 and 23800 by measuring the limiting current at isolated microelectrodes using a ferri-cyanide/ferrocyanide redox couple. Using the same technique, Hanratty [66] reported that Λ_y^+ varied between 280 and 410 (not monotonically) for Reynolds numbers between 8700 and 50200. He estimated $\Lambda_y^+ \cong 350$ over this range. These values correspond to $\Lambda_z=160 \mu\text{m}$ and $\Lambda_y=5000 \mu\text{m}$ at $\text{Re}=3000$ and $\Lambda_z=50 \mu\text{m}$ and $\Lambda_y=1500 \mu\text{m}$ at $\text{Re}=12000$ using the physical properties of our electrolyte.

Turbulence intensity adjacent to the electrode is defined by

$$\text{Turbulence intensity} = (\sqrt{(I - \bar{I})^2})/\bar{I} \quad (3.32)$$

where $\bar{I}$ is the time-averaged current and I is the instantaneous current from a single electrode. The intensity of the fluctuations in Figure 3.20 is plotted against Reynolds number in Figure 3.23. The intensity reaches its highest value of 0.093 at Re of 12200. The literature

values suggest that the turbulence intensity attains a constant value of approximately 0.1 at higher Reynolds numbers as long as the intensities are corrected for signal averaging. The smaller the microelectrode, the less signal averaging there will be. Mitchell and Hanratty [68] corrected for signal averaging and found that the adjusted value was constant at 0.1 for Reynolds numbers of ~ 10000 to 50000 . They used rectangular electrodes of two sizes: $75\ \mu\text{m} \times 825\ \mu\text{m}$ and $75\ \mu\text{m} \times 1550\ \mu\text{m}$. To correct the data at $\text{Re} \cong 10000$, the raw intensities were multiplied by about 1.2 for the $825\ \mu\text{m}$ wide electrode and by about 1.4 for the $1550\ \mu\text{m}$ wide electrode. Since our microelectrodes are much smaller, the raw signal was taken to be the actual turbulence intensity as a first approximation. Our measurements indicate that the intensity is less than 0.1 for $\text{Re} < 10000$.

Now, in light of the above values for the length scales, the time scales, and the turbulence intensities, is it surprising that the current distributions in the flow direction are correlated and that the current distributions in the transverse direction are not correlated? The turbulence intensity is large enough that the current distribution obtained after a single scan would be obscured if there were no correlation between the measured currents at the individual microelectrodes (*cf.*, Figure 4.17 in Chapter 4). The time required to sample 11 microelectrodes in the direction of flow is 17.6 ms. For comparison, Λ_t was 22.5 ms, 11.5 ms, and, 5.5 ms at $\text{Re}=5000$, 9100, and 12200, respectively. Hence, 17.6 ms is not fast enough to measure the instantaneous current distribution. It is somewhat surprising, then, that the current distribution in the direction of flow is very consistent from scan to scan. The distance spanned by the 11 microelectrodes in the flow direction and the 11 microelectrodes in the transverse direction are both $675\ \mu\text{m}$. For comparison, the Λ_z values in the transverse direction were $160\ \mu\text{m}$ at $\text{Re}=3000$ and $50\ \mu\text{m}$ at $\text{Re}=12000$. Hence, the length scale of the turbulence in the transverse direction is smaller than the distance spanned by the microelectrodes, and it is not surprising that the current measurements were not correlated in the transverse direction. In contrast, the Λ_y values in the flow direction were $5000\ \mu\text{m}$ at $\text{Re}=3000$ and $1500\ \mu\text{m}$ at $\text{Re}=12000$. Hence, the length scale of the turbulence in the flow direction is larger than the distance spanned by the microelectrodes, and, aside from

the time scales, it is not surprising that the currents measured in the flow direction were correlated.

Chapter 4

Mass Transport around Single and Multiple Cylindrical, Insulating Protrusions: Experimental and Numerical Results

4.1 Introduction

As described in Chapter 1, the precursor to the formation of zinc striations is a randomly nucleated deposit. Although the striations form only at low fractions of the limiting current where mass-transfer effects are minimal, it is tempting to suggest that localized mixing around these nuclei (or protrusions) results in enhanced mass transport in the regions where zinc is preferentially deposited. Observations from *in-situ* video microscopy [4] suggest that the zinc deposit propagates most rapidly in the wake region. Hence, if striations form as a result of enhanced mass transport of zinc from localized mixing, the mixing should act to enhance mass transport in the wake of the nuclei. In this chapter, experimental local mass-transfer rates around single, isolated protrusions and around a single

protrusion within a staggered protrusion array are presented to determine which regions around a protrusion (the wake, the front, or the sides) are, indeed, most favored for mass transport. Electrically insulated cylindrical protrusions, approximately 50 μm tall, were used as the flow disturbances. Also, theoretical mass-transport distributions around a single, insulating cylindrical protrusion are presented. The theoretical results were calculated using a commercially available finite-element program called FIDAP.

It was estimated in Chapter 1 that zinc nuclei propagate into striations even for protrusion Reynolds numbers, Re_p (see equation 1.1), on the order of 1 or less. For a 16 μm tall zinc nucleus located 7.25 cm from the center of a disk rotating at 800 RPM (laminar flow), Tsuda [1] calculated a protrusion Reynolds number of 0.95. However, in turbulent flows, where the shear rate at the surface is high, protrusion Reynolds numbers on the order of 10 may occur. Faltemier [2] noted that striations grow more rapidly and are more clearly defined at higher flow rates. To incorporate fully the effects of low and high flow rates, a Reynolds-number range of 0.56 to 127 was chosen for the experiments. The bulk fluid flow was laminar for $0.56 < \text{Re}_p < 3.64$ and turbulent for $13 < \text{Re}_p < 127$. The Reynolds numbers covered by the numerical simulations was 0.56 to 5.

4.2 Summary of experiments

The single-protrusion and protrusion-array experiments are summarized in Tables 4.1 and 4.2, respectively. The summary includes the estimated values for the physical properties of the electrolyte at 30 °C, the dimensions of the protrusions, the concentration of species in the electrolyte, and the Reynolds numbers covered in the experiment. The viscosity of water at 30 °C was used, the density of the electrolyte was assumed to be 1 g/cm³, and the measured diffusivity of Fe^{3+} ions at 25.6 °C (see Section 3.4.4) was corrected to 30 °C using the Stokes-Einstein equation:

$$\text{constant} = \frac{D_a \mu}{T} . \quad (4.1)$$

The Schmidt number of the electrolyte based on these properties is 1615.

Table 4.1: Summary of the single-protrusion experiments: physical properties and experimental conditions (wafer 6).

protrusion height (h) = 48 μm protrusion radius at base = 47 μm protrusion radius at top (r_{cyl}) = 41.5 μm viscosity* (μ) = 0.007975 g/(cm·s) density (ρ) = 1 g/cm ³ diffusivity** (D_a) = 4.938×10^{-6} cm ² /s Sc = 1615 [Fe ₂ (SO ₄) ₃] = 0.0255 M [FeSO ₄] = 0.05 M [H ₂ SO ₄] = 0.5 M	
Reynolds Number*** based on flow channel width (Re)	Reynolds number based on protrusion height (Re _p)
250	0.56
880	1.92
1500	3.38
3200	12
8600	69
12000	126

* The viscosity of water at 30 °C.

** The diffusivity of Fe³⁺ ions calculated in Chapter 3 and corrected to a temperature of 30°C using the Stokes-Einstein equation.

*** Reynolds number estimated using physical properties at 30 °C.

For each experiment, there are two Reynolds numbers that characterize the flow. The first is the Reynolds number based on the flow-channel width, Re , defined in equation 3.1. The second is the Reynolds number based on the height of the protrusion, Re_p defined in equation 1.1. Based on these Reynolds numbers, the approximate range covered in the experiments was $0.5 < Re_p < 130$ or $250 < Re < 12000$. These Reynolds numbers were calculated with the estimated electrolyte properties at 30 °C. When $Re > 2100$, the bulk fluid flow was turbulent. About half of the measurements reported in Tables 4.1 and 4.2 were measured in the laminar flow regime and half in the turbulent flow regime.

Table 4.2: Summary of the protrusion-array experiments: physical properties and experimental conditions (wafer 8).

protrusion height (h) = 50 μm protrusion radius at base = 47.5 μm protrusion radius at top (r_{cyl}) = 41.5 μm viscosity* (μ) = 0.007975 g/(cm·s) density (ρ) = 1 g/cm ³ diffusivity** (D_a) = 4.938×10^{-6} cm ² /s Sc = 1615 [Fe ₂ (SO ₄) ₃] = 0.025 M [FeSO ₄] = 0.05 M [H ₂ SO ₄] = 0.5 M	
Reynolds Number*** based on flow channel width (Re)	Reynolds number based on protrusion height (Re _p)
250	0.59
880	2.09
1500	3.64
3200	13
5700	36
8500	74
12000	127

* The viscosity of water at 30 °C.

** The diffusivity of Fe³⁺ ions calculated in Chapter 3 and corrected to a temperature of 30 °C using the Stokes-Einstein equation.

*** Reynolds number estimated using physical properties at 30 °C.

Unfortunately, the temperature of the electrolyte was not constant during these experiments since the heat exchanger (see Figure 3.12) was not installed into the flow loop until the no-protrusion experiments were performed. At the time of the measurements, the temperature of the electrolyte was monitored at the point of the electrolyte reservoir, and the average temperature was estimated to be about 30 °C. At lower flow rates, the electrolyte was heated to higher temperatures probably because the residence time in the centrifugal pump was longer. After the temperature probes were installed next to the flow cell, it was estimated that the maximum temperature was approximately 38 °C. The effect of

higher temperatures is to decrease the viscosity and, according to equation 4.1, to increase the diffusivity. From equation 3.14, the theoretical background current is proportional to diffusivity to the 2/3 power. Then, from a simple order-of-magnitude calculation, the background current is estimated to be approximately 15% higher at 38 °C than at 30 °C.

As a result, the background current was not known accurately unless it could be directly measured during the experiments. For the single-protrusion experiments, the background current was estimated from measurements at the microelectrodes located the farthest upstream. For these experiments, the data were normalized by the background current. Because similar estimates could not be obtained for the protrusion-array experiments, these data were not normalized. However, the theoretical background current density, based on the electrolyte properties at 30 °C, was plotted with the data.

The protrusions were about 48 μm tall for the single-protrusion experiment and about 50 μm tall for the protrusion-array experiment. The tops of the protrusions extended beyond the theoretical mass-transfer boundary layer (in the absence of protrusions), but the boundary layer was on the order of the protrusion height for the lowest Reynolds numbers that were studied. The boundary layer thickness, δ_m , is given in Table 4.3 for different Reynolds numbers. $Y = 0.215$ cm and $Y = 0.285$ cm correspond to the beginning and end of the measurement domain, respectively.

Re_p/Re	δ_m at $Y = 0.215$ cm	δ_m at $Y = 0.285$ cm
0.56/250	32.7 μm	36.0 μm
1.92/880	21.7 μm	23.9 μm
3.38/1500	18.0 μm	19.8 μm
12/3200	11.5 μm	12.8 μm
69/8600	6.6 μm	7.2 μm
126/12000	5.3 μm	5.9 μm

Reynolds numbers at the beginning and end of the measurement domain. δ_m is defined to

be

$$\delta_m = \frac{nF\bar{C}_a D_a}{i} \quad (4.2)$$

where the local current density, i , is given by equation 3.14 (with β in equation 3.14 determined using either equation 3.18 or 3.27 depending on whether the bulk fluid flow is laminar or turbulent). The edge of the boundary layer corresponds to roughly $C_a = 0.85\bar{C}_a$.

As described in Chapter 3, the protrusions are approximately cylindrical in shape except that the radius of the protrusions was slightly larger at the base ($\sim 47 \mu\text{m}$) than at the top ($\sim 41.5 \mu\text{m}$). The side walls of the protrusions, however, are nearly vertical, and the difference between the base and top radii is mainly due to a ring of polyimide around the base (see Figure 3.1). Hence, the radius of the protrusions, r_{cyl} , is taken to be the top radius. r_{cyl} is used for normalizing distances and for the radius of the protrusion in the numerical simulations described below. The protrusion radius, a , defined in Chapter 2 is for a protrusion with perfectly vertical side walls.

4.3 Summary of numerical calculations

The single-protrusion case was modeled for the lower Reynolds numbers, where the bulk fluid flow is laminar, using a commercially available finite-element code called FIDAP, a product of Fluid Dynamics International, Inc. The numerical simulations are summarized in Table 4.4. The summary includes the physical parameters, the dimensions of the protrusion, and the Reynolds numbers used in the study. The simulations for $\text{Re}_p = 1$, 3, and 5 were done initially to learn how to do the simulations, and the simulations at $\text{Re}_p = 0.56$, 1.92, and 3.38 were done afterwards to match the experimental conditions. The protrusion radius was set to $r_{\text{cyl}} = 41.5 \mu\text{m}$, and the protrusion height was set to $h = 48 \mu\text{m}$. The corners of the protrusion were given a radius of curvature of $0.1r_{\text{cyl}}$ or $4.15 \mu\text{m}$. It was feared that sharp corners may lead to numerical inaccuracies, but these fears were probably unfounded. The physical parameters were chosen to be constant and to be the same as the physical parameters estimated for the experiments at 30°C .

Table 4.4: Summary of the numerical simulations for predicting local mass-transport rates. Only the single-protrusion case is modeled and the bulk fluid flow is laminar.

$C_a = 0.05 \text{ M}$
$\rho = 1 \text{ g/cm}^3$
$\mu = 0.007975 \text{ g/(cm}\cdot\text{s)}$
$D_a = 4.938 \times 10^{-6} \text{ cm}^2/\text{s}$
$Sc = 1615$
$r_{\text{cyl}} = 41.5 \text{ }\mu\text{m}$
$h = 48 \text{ }\mu\text{m}$
$Re_p = 0.56, 1, 1.92, 3, 3.38, 5$

A surface projection of the discretized domain (the mesh) is shown in Figure 4.1, and an expanded view of the mesh near the protrusion is shown in Figure 4.2. 15729 nodes were used for the discretization with linear basis functions to approximate the local velocity or concentration profile. The surface projection shows the inflow plane, the symmetry plane, the electrode plane, and the protrusion itself. Only half of the protrusion needed to be meshed because of the plane of symmetry. An outflow plane, side plane, and top plane, in that order, lie opposite the above-mentioned planes, but they are not shown in the figure. The mesh extends for $12 r_{\text{cyl}}$ upstream and downstream of the protrusion, $12 r_{\text{cyl}}$ transverse of the protrusion, and $6 r_{\text{cyl}}$ vertically away from the electrode. For comparison, the leading edge of the electrode lies about $60.2 r_{\text{cyl}}$ upstream of the protrusion. The Y -position corresponding to the position of the inflow plane is $Y = 0.2002 \text{ cm}$ while the position of the outflow plane corresponds to $Y = 0.2998 \text{ cm}$. To account for the missing electrode length between 0 cm and 0.2002 cm , appropriate mass-transfer boundary conditions are needed on the domain boundaries.

The boundary conditions are summarized in Table 4.5. The velocity was set to zero at the electrode and on the protrusion, to a linear-shear flow on the inflow and side planes, and to $6 r_{\text{cyl}} \beta$ on the top plane. No velocity condition was required by FIDAP on the outflow plane. After applying these conditions, the full Navier-Stokes equations were solved separately from the mass-transfer problem. Although the domain was finite, the resultant velocity profile should be similar to the velocity profile in an infinite domain because the

Figure 4.1: A surface projection of the FIDAP mesh. The inflow, symmetry, and electrode planes are shown in addition to the protrusion itself.

Figure 4.2: A closeup of the mesh used for FIDAP near the protrusion.

Table 4.5: The fluid-flow and mass-transport boundary conditions for the FIDAP simulations.

Plane	Velocity boundary condition	Mass-transfer boundary condition
Inflow	$u_x = 0$ $u_y = \beta x$ $u_z = 0$	Equation 3.10 with $Y = 0.2002$ cm
Outflow	None*	Zero diffusive flux
Electrode	$u_x = 0$ $u_y = 0$ $u_z = 0$	$C_a = 0$
Top	$u_x = 0$ $u_y = \beta(6R)$ $u_z = 0$	$C_a = \bar{C}_a$
Symmetry	$\frac{du_y}{dz} = 0$ $u_z = 0$	$\frac{dC_a}{dz} = 0$
Side	$u_x = 0$ $u_y = \beta x$ $u_z = 0$	$\frac{dC_a}{dz} = 0$
Protrusion	$u_x = 0$ $u_y = 0$ $u_z = 0$	$\frac{dC_a}{dn} = 0$ (n is the normal direction)

*One or more boundary condition is required. It must be automatically applied by FIDAP.

wall shear was determined to recover to 98% of its value at infinity 7.34 cylinder radii upstream/downstream of a protrusion with an aspect ratio of $h/a=1$ from the boundary-integral technique (*cf.*, Table 2.2). The protrusion discretized in FIDAP has an $h/r_{\text{cyl}}=1.16$.

Next, the mass-transfer boundary conditions in Table 4.5 were applied. Only a single species "a" was considered, where species "a" represents the Fe^{3+} ions. The concentration profile obtained from the Lvque solution (equation 3.10) was applied at the inflow plane using $Y=0.2002$ cm, $D_a = 4.938 \times 10^{-6}$, and a β corresponding to the Reynolds number. By doing this, it is assumed that the protrusion does not influence mass transfer farther than $12r_{\text{cyl}}$ upstream of the protrusion. The diffusive flux was set to zero on the outflow plane, the symmetry plane, the side plane, and the protrusion. The concentration of species "a" was set to zero on the electrode and to its bulk value of 0.05 M on the top

plane. After applying the boundary conditions, the full convective-diffusion equation was solved.

The relative sizes of the mass-transport boundary layer, the FIDAP solution domain, and the protrusion are shown from a side view in Figure 4.3 for $Re_p=1$ and $Sc=1615$. The vertical scale is magnified by a factor of 9.4 relative to the horizontal scale. The velocity profile along the plane $Z/W = 0.5$ of a $0.3175 \text{ cm} \times 0.3175 \text{ cm}$ square duct (the dimensions of our flow cell in cross section) is shown in comparison to the linear velocity profile applied to the inflow and side planes of the FIDAP solution domain. The linear velocity profile provides an excellent approximation to the actual velocity profile in the vicinity of the mass-transport boundary layer and the protrusion. Note that the velocity profile is assumed to be constant in the transverse or Z direction. This assumption should introduce negligible error because the mass-transport distribution in a square duct in the absence of protrusions, which is proportional to $\beta^{1/3}$, varies by only 1% in the transverse direction over the distance spanned by the microelectrodes (see Figure 3.18).

To calculate a theoretical microelectrode current, the positions of the microelectrodes relative to the elements in the mesh are needed. The outline of the microelectrodes are superimposed on the electrode plane of the mesh in Figure 4.4. The microelectrodes that lie in the flow direction are cut in half by the symmetry plane. Since the flux calculated by FIDAP is a constant over each element, the theoretical current to any particular microelectrode is the sum of the fluxes to the elements that overlap the microelectrode weighted by the fractional area of the elements that overlap the microelectrode.

4.4 Mass transport around single protrusions in laminar flow: experimental and numerical results

In this section, the theoretical and experimental dimensionless microelectrode currents are compared first for a single insulating protrusion. Next, for the same protrusion geometry, the theoretical dimensionless current to individual elements in the FIDAP mesh

Figure 4.3: A diagram showing the relative position and sizes of the mass-transfer boundary layer (computed under the conditions $Re_p=1$ and $Sc=1615$), the protrusion, and the FIDAP solution domain. The scale in the vertical direction is expanded by a factor of 9.4. The velocity profile along the plane $Z/W = 0.5$ of a $0.3175 \text{ cm} \times 0.3175 \text{ cm}$ square duct is shown in comparison to the linear velocity profile applied on the inflow and side plane of the FIDAP solution domain.

Figure 4.4: The outline of the microelectrode superimposed on the electrode plane of the FIDAP mesh. The microelectrodes that lie in the direction of flow are cut in half at the z -position of the symmetry plane. The microelectrodes are outlined using thick lines, and the mesh is drawn using thin lines.

is presented in addition to theoretical concentration contours. As is evident from Figure 4.4, the current distribution from the elements in the FIDAP mesh is more detailed than the current distribution from the microelectrodes. Also, the elements, unlike the microelectrodes, go to the very edge of the protrusion.

The theoretical and experimental dimensionless currents to the microelectrodes are plotted against dimensionless electrode distance for $Re_p=0.56$, 1.92, and 3.38 in Figures 4.5 to 4.7. The polyimide protrusion is located at $(y,z)=(0,0)$. The top plot in each figure shows the current distributions in the flow direction, and the bottom plot shows the current distribution in the transverse direction. The current is normalized by the background current, I_0 , and distances are normalized by r_{cyl} . The closest microelectrode to the protrusion is located at $2.41 r_{cyl}$, and the farthest microelectrode from the protrusion is located at $8.43 r_{cyl}$. The lines represent the theoretical current distribution calculated using FIDAP, and the symbols represent the experimental current distribution. The filled symbols are data taken with the electrolyte flowing in the AS-direction, and the unfilled symbols are data taken with the electrolyte flowing in the S-direction. Each data symbol represents a measurement from a single scan.¹

For the experiments, I_0 is determined separately for each data scan. The currents to the 2 microelectrodes that are located the farthest upstream (microelectrodes 1 and 2 with the flow in the S-direction and microelectrodes 10 and 11 with the flow in the AS-direction—see Figure 3.6) are assumed to be undisturbed by the presence of the protrusion. The background current measured at any one of these microelectrodes can be used to determine the background current at the remaining microelectrode positions because the local current is inversely proportional to $Y^{1/3}$ in the flow direction and directly proportional to $\beta^{1/3}$ in the transverse direction (*cf.*, equations 3.14 and 3.18). When the flow is in the S-direction, for example, two background current distributions are determined separately from the currents to microelectrodes 1 and 2. These two background current distributions

¹As described in Chapter 3, in a single data scan, the 22 microelectrodes are sampled by the multiplexer in 17.6 ms.

Figure 4.5: The experimental current distribution around a single polyimide protrusion at $Re_p = 0.56$ in (a) the flow direction and (b) the transverse direction compared to the theoretical current distribution computed using FIDAP. The protrusion is positioned at $(y, z) = (0, 0)$.

Figure 4.6: The experimental current distribution around a single polyimide protrusion at $Re_p = 1.92$ in (a) the flow direction and (b) the transverse direction compared to the theoretical current distribution computed using FIDAP. The protrusion is positioned at $(y, z) = (0, 0)$.

Figure 4.7: The experimental current distribution around a single polyimide protrusion at $Re_p = 3.38$ in (a) the flow direction and (b) the transverse direction compared to the theoretical current distribution computed using FIDAP. The protrusion is positioned at $(y, z) = (0, 0)$.

are then averaged and used to normalize the current to the other microelectrodes.

The experimental current distributions with the electrolyte flowing in the S- and AS-directions agree closely in Figures 4.5 to 4.7. The S-direction data lie slightly above the AS-direction data downstream of and to one side ($z < 0$) of the protrusion, but the discrepancy is only about $I/I_0 = 0.02$ even in these regions. Also, the theoretical current distributions agree well with the experimental current distributions. However, the theoretical currents to the microelectrodes nearest to the polyimide protrusion, in both the flow and transverse directions, tend to be higher than the corresponding experimental currents. The error is the greatest at these microelectrodes because the current distribution changes the most rapidly close to the protrusion.

Mass transport is inhibited over the area spanned by the microelectrodes in Figures 4.5 to 4.7 (neglecting the small enhancement at $y = 8.43 r_{\text{cyl}}$ for $\text{Re}_p = 0.56$). Also, the dimensionless current is always the lowest at the closest microelectrode to the protrusion in the wake, and the mass-transport distribution on either side of the protrusion is symmetric. The dimensionless current relaxes to unity at about $y = -5 r_{\text{cyl}}$ upstream of the protrusion and at about $z = \pm 6 r_{\text{cyl}}$ to either side of the protrusion. Downstream of the protrusion, the dimensionless current also approaches unity, but there are still small mass-transfer effects past $8.43 r_{\text{cyl}}$. At $y = 8.43 r_{\text{cyl}}$, the dimensionless current is slightly greater than unity for $\text{Re}_p = 0.56$, and slightly less than unity for $\text{Re}_p = 1.92$ and 3.38 for both the theoretical and the experimental mass-transport distributions.

The experimental dimensionless currents are superimposed in Figure 4.8 for $\text{Re}_p = 0.56$, 1.92 , and 3.38 . The top graph shows the current distribution in the direction of flow, and the bottom graph shows the current distribution in the transverse direction. For the microelectrodes immediately adjacent to the protrusion, the current increases monotonically upstream and to either side of the protrusion and decreases monotonically in the wake of the protrusion. The monotonic trend in the wake is broken at $y = 8.43 r_{\text{cyl}}$. At this position, the Reynolds numbers in the order of decreasing current density are $\text{Re}_p = 0.56$, 3.38 , and 1.92 , but the currents for $\text{Re}_p = 1.92$ and 3.38 are nearly identical. This break in the mono-

Figure 4.8: The experimental current distribution at $Re_p = 0.56, 1.92$, and 3.38 in (a) the flow direction and (b) the transverse direction. The S-direction and AS-direction data are superimposed and are represented by the same data symbol at a given Reynolds number.

tonic trend is confirmed by the theoretical microelectrode current distributions shown in Figure 4.9 for $Re_p = 5, 0.56, 3.38$, and 1.92 (listed in the order of decreasing current density at $y = 8.43 r_{cyl}$ in the wake). The current is close to a minimum for $Re_p = 1.92$ and 3.38 . Farther downstream, the current densities should approach $I/I_0 = 1$.

The dimensionless current distributions from the individual elements in the FIDAP mesh are presented in Figure 4.10 ($Re_p = 1$), Figure 4.11 ($Re_p = 3$), and Figure 4.12 ($Re_p = 5$). In each of these figures, the scale is the same, and an inset graph shows an expanded view of the current distribution within 1 cylinder radius of the protrusion. The dimensionless current is plotted against dimensionless radial distance, σ/r_{cyl} , for $\phi = 0, 45, 90, 135$, and 180 , where the downstream direction corresponds to $\phi = 0$ and the upstream direction corresponds to $\phi = 180$ (see Figure 2.3 for the coordinate system). A straight line drawn at these angles coincides with element edges on the electrode plane of the mesh (see Figure 4.4). For example, for the line at $\phi = 45$, one element lies on either side of the line at any given radial position. The currents to these two elements are averaged (weighted by the element areas), and the location of the average current is taken to be at $\phi = 45$ and the average radial position of the elements. The radial position of an element is its center. For $\phi = 0$ or 180 , imaginary elements can be assumed to exist on the opposite side of the symmetry plane.

Figures 4.10 to 4.12 reveal a maximum in the dimensionless current immediately in front of the protrusion and a global minimum in the dimensionless current immediately behind the protrusion. The maximum increases from 1.51 at $Re_p = 1$ to 3.21 at $Re_p = 5$ whereas the minimum decreases from 0.248 at $Re_p = 1$ to 0.0979 at $Re_p = 5$. Upstream from the maximum ($1.70 r_{cyl}$ at $Re_p = 1$ and $1.94 r_{cyl}$ at $Re_p = 5$), there is a local minimum in the dimensionless current which is less distinct at the higher Reynolds numbers. The location and magnitudes of the minima and maxima are listed Table 4.6. At all angles except $\phi = 0$ (downstream), the dimensionless current relaxes to unity within the limits of the computational domain. At $\phi = 0$ and $10.5 r_{cyl}$, the dimensionless current exceeds unity for $Re_p = 1$ (just barely) and for $Re_p = 5$. The dimensionless currents should become unity

Figure 4.9: The theoretical dimensionless current densities to the microelectrodes at $Re_p = 0.56, 1.92, 3.38$, and 5 plotted against dimensionless distance in (a) the flow direction and (b) the transverse direction.

Figure 4.10: The theoretical current distribution in the radial direction at $\phi=0^\circ$, 45° , 90° , 135° , and 180° . The current distribution was calculated using FIDAP under the conditions $Re_p = 1$ and $Sc=1615$.

Figure 4.11: The theoretical current distribution in the radial direction at $\phi=0^\circ, 45^\circ, 90^\circ, 135^\circ$, and 180° . The current distribution was calculated using FIDAP under the conditions $Re_p = 3$ and $Sc=1615$.

Figure 4.12: The theoretical current distribution in the radial direction at $\phi=0^\circ$, 45° , 90° , 135° , and 180° . The current distribution was calculated using FIDAP under the conditions $Re_p = 5$ and $Sc=1615$.

Table 4.6: The location* and magnitudes of minima and maxima in the theoretical dimensionless current for $Re_p=1, 3$, and 5 .

Re_p	Global maximum	Global minimum	local minimum
1	$I/I_0=1.51$	$I/I_0=0.248$	$I/I_0=0.761$
	$\phi=180$	$\phi=0$	$\phi=180$
	$\sigma/r_{cyl}=1.12$	$\sigma/r_{cyl}=1.12$	$\sigma/r_{cyl}=1.70$
3	$I/I_0=2.59$	$I/I_0=0.153$	$I/I_0=0.869$
	$\phi=180$	$\phi=0$	$\phi=180$
	$\sigma/r_{cyl}=1.12$	$\sigma/r_{cyl}=1.12$	$\sigma/r_{cyl}=1.82$
5	$I/I_0=3.21$	$I/I_0=0.0979$	$I/I_0=0.918$
	$\phi=180$	$\phi=0$	$\phi=180$
	$\sigma/r_{cyl}=1.12$	$\sigma/r_{cyl}=1.04$	$\sigma/r_{cyl}=1.94$

*The three significant figures for the radial position refer to the radial position of the element on which the maximum or minimum was found.

farther downstream.

The insulating protrusion impedes mass transport over a large area compared to the area over which mass transport is enhanced. The net effect of the protrusion on mass transport over the FIDAP computational domain is given by the total dimensionless currents in Table 4.7. These dimensionless currents were determined by calculating the

Table 4.7: The total dimensionless current to the electrode in the FIDAP computational domain. The total dimensionless current is determined by computing the total current to the electrode in the FIDAP domain and dividing this by the total background current to the same electrode area including the area of the electrode normally covered by the protrusion.

Reynolds number (Re_p)	Total dimensionless current
1	0.98305
3	0.98316
5	0.98371

total current to the electrode area in the FIDAP domain and normalizing it by the total background current (Section 3.4) to an equivalent electrode area in addition to the electrode

area normally covered by the protrusion. In each case ($Re_p=1, 3, 5$), the total dimensionless current is approximately 0.98, which means that mass transport is slightly attenuated over the FIDAP domain.

The net effect of the protrusion over an infinite domain, however, is up to conjecture. Since the local dimensionless current at $\phi = 0$ and $10.5 r_{cyl}$ exceeds unity for $Re_p=1$ and $Re_p=5$ (the dimensionless current probably exceeds unity for $Re_p=3$ farther downstream), the ions that would normally react in the absence of a protrusion probably react at the electrode farther downstream. If this is true, then the protrusion redistributes the reaction instead of altering the total mass flux.

Contours of constant dimensionless concentration, $C_a/\bar{C}_a$, near the protrusion are plotted in Figure 4.13 ($Re_p = 1$), Figure 4.14 ($Re_p = 3$), and Figure 4.15 ($Re_p = 5$). The same contours are plotted over the entire domain in Figure 4.16. The contours are drawn on the symmetry plane and on the protrusion, and they are viewed from the vantage point of an observer slightly above the protrusion and facing the symmetry plane. $C_a/\bar{C}_a$ is 0.05 for the bottom-most contours and 0.95 for the top-most contours where the increment between adjacent contours is 0.1. The closed contours above the 0.95 contour are numerical artifacts and should be ignored. The dashed line is the theoretical contour for $C_a/\bar{C}_a = 0.95$ when no protrusion is present. At the inflow plane, this contour is forced to coincide with the top-most contour by the boundary conditions. The downward-pointing triangles mark the location of a local minimum in the mass flux and the upward-pointing triangles mark the location of a local maximum in the flux.

High-flux regions occur where the concentration contours are tightly spaced such as immediately in front of the protrusion near the electrode and immediately behind the protrusion away from the electrode. Similarly, low-flux regions occur where the concentration contours are widely spaced such as near the electrode in the wake.

As the Reynolds number increases, the mass-transport boundary layer decreases in thickness. For $Re_p=3$ and 5, the depleted electrolyte in the boundary layer is swept to the top of the protrusion in the wake where it is exposed to bulk electrolyte, but the depleted

Figure 4.13: Contours of constant dimensionless concentration, $C_a/\bar{C}_a$, near to the protrusion for $Re_p = 1$ on the inflow plane and on the protrusion. The minimum contour is $C_a/\bar{C}_a = 0.05$, the maximum contour is $C_a/\bar{C}_a = 0.95$, and the increment between each is 0.1. The dashed line is for $C_a/\bar{C}_a = 0.95$ when no protrusion is present. The downward-pointing triangles are positioned at local mass transport minima, and the upward-pointing triangles are positioned at local mass-transport maxima.

Figure 4.14: Contours of constant dimensionless concentration, $C_a/\bar{C}_a$, near the protrusion for $Re_p = 3$ on the inflow plane and on the protrusion. The minimum contour is $C_a/\bar{C}_a = 0.05$, the maximum contour is $C_a/\bar{C}_a = 0.95$, and the increment between each is 0.1. The dashed line is for $C_a/\bar{C}_a = 0.95$ when no protrusion is present. The downward-pointing triangles are positioned at local mass transport minima, and the upward-pointing triangles are positioned at local mass-transport maxima.

Figure 4.15: Contours of constant dimensionless concentration, $C_a/\bar{C}_a$, near the protrusion for $Re_p = 5$ on the inflow plane and on the protrusion. The minimum contour is $C_a/\bar{C}_a = 0.05$, the maximum contour is $C_a/\bar{C}_a = 0.95$, and the increment between each is 0.1. The dashed line is for $C_a/\bar{C}_a = 0.95$ when no protrusion is present. The downward-pointing triangles are positioned at local mass transport minima, and the upward-pointing triangles are positioned at local mass-transport maxima.

Figure 4.16: Contours of constant dimensionless concentration, $C_a/\bar{C}_a$, for $Re_p = 1, 3$, and 5 viewed over the entire domain.

electrolyte is not swept above the protrusion. Farther downstream of the protrusion, the mass-transfer boundary layer slowly relaxes to its undisturbed thickness.

4.5 Mass transport around single protrusions in turbulent flow

In this section, experimental current distributions around single protrusions are presented for the case where the bulk fluid flow was turbulent. Theoretical results were not calculated in the turbulent regime. As discussed in Section 3.5, the current distributions were obtained only in the bulk flow direction because the current distribution for a single scan closely resembled the final time-averaged current distribution. The unnormalized, raw current distributions around a single protrusion are shown in Figure 4.17 for $Re_p=12$, 69, and 126. The current distributions for the individual scans are, indeed, very similar, but they are displaced in magnitude.

The corresponding normalized current distributions are shown in Figure 4.18. Each scan was normalized separately using the same procedure described in Section 4.4 for the laminar-flow data. Upstream of the protrusion, the solid line is drawn through the average dimensionless current at each microelectrode position. Downstream of the protrusion, however, the S-Direction and AS-direction current distributions must be aligned in order to draw a relatively smooth curve through the data points (see especially $Re_p=126$). The data points in the two flow directions were shifted vertically by equal and opposite amounts and a line then was drawn through the resulting average dimensionless current at each microelectrode position. The unshifted data symbols are drawn on the graph.

Upstream of the protrusion, the current distribution is nearly constant except very close to the protrusion. At $Re_p=69$ and 126, a sharp spike in the current is measured at the closest microelectrode to the protrusion. Presumably, this spike also exists at $Re_p=12$, but it occurs closer than $1.81 r_{cyl}$ from the protrusion center.² The spike is about $1.4 I/I_0$

²The center-to-center distance between the closest microelectrode and the protrusion is $2.41 r_{cyl}$, but the

Figure 4.17: Unnormalized current distributions in the direction of flow for a single protrusion located at $y=0$ when the bulk fluid flow is turbulent: (a) $Re_p=12$, (b) $Re_p=69$, (c) $Re_p=126$. Each data symbol is a measurement from a single scan. The filled symbols were collected with the electrolyte flowing in the AS-direction, and the unfilled symbols were collected with the electrolyte flowing in the S-direction. Lines connect connect data symbols from the same scan.

Figure 4.18: Normalized current distributions in the direction of flow for a single protrusion located at $y=0$ when the bulk fluid flow is turbulent: (a) $Re_p=12$, (b) $Re_p=69$, (c) $Re_p=126$.

at $Re_p=69$ and about $1.5 I/I_0$ at $Re_p=126$.

In the wake, the dimensionless current increases with increasing downstream distance. The rate of increase levels off near the end of the measurement domain to values which are clearly greater than unity: $1.1 I/I_0$ for $Re_p=12$ and $1.5 I/I_0$ for $Re_p=69$ and 126 . For $Re_p=126$, the current actually decreases for a short distance at $y=4 r_{cyl}$. It is not clear whether this decrease is real or whether it results from an artifact in the measurement device. For $Re_p=12$, the lowest dimensionless current was measured in the wake of the protrusion, similar to the laminar-flow measurements. For $Re_p=69$ and 126 , however, the lowest dimensionless current was the undisturbed upstream flux. However, it is possible that the dimensionless current in the wake, very close to the protrusion, falls below unity for $Re_p=69$ and 126 . For $Re_p=69$ and 126 , the insulating protrusion appears to increase the total mass flux in the vicinity of the protrusion.

4.6 Summary of the single-protrusion experimental results in the direction of flow

The dimensionless current distributions measured around a single insulating protrusion are summarized in Figure 4.19 (upstream of the protrusion) and Figure 4.20 (downstream of the protrusion) for $Re_p=0.56$ to 126 . The current distributions were determined by drawing curves through the data as described in Section 4.5 paragraph 2.

In Figure 4.19, at the lower Reynolds numbers, mass transport is inhibited at the microelectrodes up to $5 r_{cyl}$ upstream of the protrusion. The dimensionless current increases with increasing Reynolds number until there is no detectable mass-transfer decrease upstream of the protrusion at $Re_p=69$. At $Re_p=69$ and 126 , a large increase in the dimensionless current ($1.4 I/I_0$ at $Re_p=69$ and $1.5 I/I_0$ at $Re_p=126$) is measurable at $y=-2.41 r_{cyl}$. The numerical results showed that a large increase in the current also occurs upstream of the protrusion for $1 \leq Re_p \leq 5$, but the increase occurs too close to edge of this electrode is $1.81 r_{cyl}$ away.

Figure 4.19: The superimposition of the dimensionless current distributions upstream of the protrusion for $Re_p=0.56$ to 126.

Figure 4.20: The superimposition of the dimensionless current distributions downstream of the protrusion for $Re_p=0.56$ to 126.

the protrusion to be detectable by our measurement device. Presumably, the the current distribution for $Re_p=12$ behaves similarly.

In Figure 4.20, the dimensionless current increases monotonically with downstream distance except for $Re_p=126$ where the dimensionless current decreases for a short distance at $y=4 r_{cyl}$. This decrease may be due to an artifact in the measurement device. For all Reynolds numbers, the rate of increase levels off near the end of the measurement domain, but the dimensionless current is still increasing at a slow rate for $Re_p=0.56$ to 12. At $Re_p=69$ and 126 it is not clear whether the dimensionless current has reached a maximum or not. Interestingly, the mass-transfer enhancement at $Re_p=69$ and 126 is approximately the same, the maximum being about $1.5 I/I_0$. This is nonintuitive because one would expect more vigorous mixing at higher Reynolds numbers and, as a result, higher dimensionless currents. However, depletion of the reactant upstream of the protrusion may also be greater at higher Reynolds numbers. The net effect may be that the dimensionless current downstream of the protrusion stays about the same between $Re_p=69$ and 126.

4.7 Experimental current distributions around a single protrusion in a protrusion array for laminar flow.

The current distributions in the flow direction are shown in Figure 4.21 around the central protrusion ($y=0, z=0$) in the protrusion array for $Re_p=0.59, 2.09$, and 3.67 . Protrusions are located every $10.8 r_{cyl}$ in the flow direction in line with the microelectrodes at $z=0$. For each Reynolds number, the lowest current densities are measured in the wakes of the protrusions at $y= -10.8 r_{cyl}$ and $y=0 r_{cyl}$. A maximum in the current occurs approximately half way between the protrusions.

In Figure 4.21, the data symbols at three adjacent microelectrode positions are circled for each Reynolds number, both upstream and downstream of the central protrusion. These data symbols are forced to be collinear by shifting the current distributions in the S- and AS-directions by equal but opposite amounts. This procedure ensured that the current

Figure 4.21: A diagram showing the method by which the current distributions in the S-direction (the unfilled data symbols) and AS-direction (the filled data symbols) are aligned for a protrusion array. Each data symbol represents a single measurement from a single scan.

Figure 4.22: The current distribution in the flow direction around a single protrusion within a protrusion array for $Re_p=0.59, 2.09, 3.67$. The bulk fluid flow is laminar. The solid line is the theoretical background current calculated using estimated physical properties at 30°C .

distributions in the S- and AS-directions would be aligned. The current distributions in the transverse direction are aligned simultaneously.

In Figure 4.22, the theoretical background current distributions (calculated using the physical properties listed in Table 4.2) are superimposed on the current distributions from Figure 4.21. The measured current was not normalized by the background current because of the uncertainty in the background current (see Section 4.2). However, if the measured current were normalized by the background current, the normalized current distribution would be periodic because the background current distribution intersects the measured current distribution at equivalent positions in the array upstream and downstream of the protrusion. Equivalent positions are positions where the normalized³ current density is the same because of periodicity or symmetry. Such positions are shown schematically in

³At higher Reynolds numbers, the current distributions are periodic before normalization. In this case, equivalent positions are defined in terms of the unnormalized current distributions.

Figure 4.23: A schematic diagram showing the equivalent positions in the protrusion array that was used for the experiments. The points "a" are at equivalent positions. There are two equivalent positions per unit cell because of the symmetry in the transverse direction.

Figure 4.23.

Figure 4.24 shows the current distribution in the transverse direction for $Re_p=0.59$, 2.09, and 3.67. The corresponding theoretical background current at each Reynolds number is nearly constant. At $Re_p=2.09$ and 3.67, two distinct maxima and one minimum are observed on either side of the central protrusion. At $Re_p=0.59$, the current distribution plateaus instead of reaching a distinct maximum. The positions and the equivalent positions of these maxima, minima, and plateaus in the protrusion array are marked in the bottom graph in Figure 4.25. The location of the maxima occur approximately at the tips of the

Figure 4.24: The current distribution in the transverse direction around a single protrusion within a protrusion array for $Re_p=0.59, 2.09, 3.67$. The solid line is the theoretical background current calculated using estimated physical properties at 30°C .

Figure 4.25: The location of current minima, maxima, and plateaus within the protrusion array measured at the microelectrodes in the transverse direction. The $\times$ symbols in the bottom graph mark the location of protrusions within the array. The locations of the maxima occur, approximately, at the tips of the lines with the double arrow heads, the minima occur at the midpoint of these lines, and the plateaus occur along these lines. The channels labeled in the diagram are defined as strips along the electrode in the direction of flow which are not covered by protrusions.

lines with the double arrow heads, the minima occur at the midpoint of these lines, and the plateaus occur along these lines. Interestingly, the maxima and the plateaus are not centered at $z/r_{\text{cyl}} = (\dots, -8.13, -2.71, 2.71, 8.13, \dots)$, where there are no protrusions in the direction of flow (marked as "channels" in the figure). One might expect the shear stress and, as a result, the mass transport to reach a local maximum along the centerline of these channels because there are no protrusions to impede the fluid motion. Instead, as Reynolds number decreases, mass transport becomes most favorable in line with the protrusions because the plateau at $Re_p = 0.59$ is centered in line with the protrusions.

The current distributions in the flow direction and the transverse direction are superimposed in Figure 4.26. The current is normalized by the background current to show that the normalized current is the same at equivalent positions (marked by the circles) in the array. At the lowest Reynolds number ($Re_p = 0.59$), the current distribution appears to be nearly identical in the flow direction and the transverse direction. At the higher Reynolds numbers ($Re_p = 2.09$ and 3.67), the current distributions in the two directions become dissimilar, where the highest dimensionless currents occur in the transverse direction.

4.8 Experimental current distribution around the central protrusion in the protrusion array for turbulent flow

In this section, experimental current distributions around the central protrusion in the protrusion array are presented for the case where the bulk fluid flow was turbulent. In the turbulent regime, current distributions in the transverse direction were not obtained (see Section 3.5), and theoretical results were not obtained. The current distributions in the S- and AS-directions were aligned by the same procedure that was used for the laminar flow experiments (illustrated in Figure 4.21). The unnormalized measured current distributions and the theoretical background current distributions in the direction of flow are shown in Figure 4.27 for $Re_p = 13, 36, 74$, and 127 . The same measured current distributions are shown in a single graph in Figure 4.28.

Figure 4.26: The dimensionless current distributions in the direction of flow and the transverse direction are superimposed for $Re_p=0.59, 2.09$. The bulk fluid flow is laminar. The currents are normalized by the theoretical background current calculated using the physical properties in Table 4.2.

Figure 4.27: The current distribution in the flow direction around the central protrusion in the protrusion array for (a) $Re_p=13$, (b) $Re_p=36$, (c) $Re_p=74$, and (d) $Re_p=127$. The bulk fluid flow is turbulent. The solid line is the background current calculated using the physical properties in Table 4.2.

Figure 4.28: The current distribution in the flow direction around the central protrusion in the protrusion array for $Re_p=13, 36, 74$, and 127 . The current distributions are the same as in Figure 4.27, but they are all shown on the same axes.

At $Re_p=13$ and 36 , the current density at equivalent microelectrode positions decreases with downstream distance at approximately the same rate as the background current density. In contrast, at $Re_p=74$ and 127 , there is no significant difference in the measured current density at equivalent microelectrode positions indicating that the current distributions have reached a steady state and are periodic before normalization. $Re_p=74$ and 127 corresponds to channel Reynolds numbers of $Re=8500$ and 12000 . At similar Reynolds numbers ($Re=7900$ and 10600), the background current density does not reach a steady state (see Figure 3.19). Hence, steady state is achieved in shorter electrode lengths at the same Reynolds numbers in the presence of the protrusion array.

As observed in the single-protrusion experiments for $Re_p=69$ and 126 , a rapid increase in the current is detectable in front of each protrusion for $Re_p=36$, 74 , and 127 . However, for the single-protrusion experiments, the mass-transport enhancement in the wake was similar to the increased mass transport in front of the protrusions. In contrast, for the protrusion array, the current densities in the wake of each protrusion are significantly lower than the current densities in front of each protrusion.

4.9 Summary of the protrusion-array experimental results in the direction of flow

For the purpose of summarizing the current distributions in the direction of flow for the protrusion array, it is convenient to choose reference currents, I_{ref} , to normalize the data. Two I_{ref} are chosen at each Reynolds number as illustrated in Figure 4.29. The two I_{ref} are measured at $y/r_{cyl}=-8.43$ and 2.41 , which are equivalent positions in the array. The current measured at $y/r_{cyl}=-8.43$ is used to normalize the currents measured upstream of the central protrusion, and the current measured at $y/r_{cyl}=2.41$ is used to normalize the currents measured downstream of the central protrusion. Then, the normalized current distributions upstream and downstream of the central protrusion were averaged at corresponding "equivalent" points to obtain a single, representative current distribution.

Figure 4.29: Replot of the data for the protrusion array in the flow direction from Figure 4.22. The marked values, I_{ref} , are used to normalize the data for the protrusion array in Figure 4.30.

The normalized current distributions are plotted in Figure 4.30 for $Re_p=0.59$ to 127. The y/r_{cyl} values on the abscissa can be converted to values corresponding to equivalent positions by subtracting or adding $y/r_{\text{cyl}}=10.84$, the distance between protrusions in the flow direction. Disregarding the sudden the current increases in front of the protrusions for $Re_p=36$, 74, and 127, the most nonuniform current distributions are between $Re_p=3.67$ and 13. At higher Reynolds numbers, the current distribution more uniform probably because of increased mixing. Interestingly, the normalized current distributions for $Re_p=74$ and 127 are nearly the same. A similar observation was made for the single-protrusion experiments for $Re_p=69$ and 126.

4.10 Discussion and conclusions

When zinc striations form during electrodeposition, the preferential deposition observed in the wake of nuclei is not caused by enhanced mass transport from localized

Figure 4.30: Summary of the current distributions in the direction of flow around the central protrusion in the protrusion array for $Re_p=0.59$ to 127. The local current is normalized by a reference current (see Figure 4.29).

mixing. The numerical and experimental results in this study indicate that the wake region behind a protrusion is the least favorable region for mass transport—with the exception of the single-protrusion case at $Re_p=69$ and 126. For this exception, the mass transfer at $y=-2.41 r_{cyl}$ (upstream of the protrusion) was comparable to the mass transfer between $y=6.02$ and $8.43 r_{cyl}$ (downstream of the protrusion). For the protrusion array, mass-transfer was always less favorable in the wake of each protrusion than in front of each protrusion. Since the protrusion array represents a randomly nucleated zinc deposit better than the single protrusion, it is unlikely that the cause of striations is related to the enhanced mass transport in the wake region observed for the single-protrusion case at $Re_p=69$ and 126. Moreover, individual zinc nuclei are observed to meld into striations at Re_p on the order of 1, well before an Re_p of 69 or 126 is attained.

Although high Reynolds numbers are not required for zinc nuclei to propagate into striations, striations form more rapidly and become more well defined with increasing Reynolds number [2]. Interestingly, the current density becomes more nonuniform within a protrusion array with increasing Reynolds number until, approximately, $Re_p=13$ (see Figure 4.30). In view of this, striations may form more quickly at higher Reynolds numbers because of increased nonuniformity in mass transport, although the mechanism is not understood. At Re_p higher than 13, increased mixing causes the mass-transport distribution to be more uniform in the array, but Re_p much higher than 10 are probably not observed during zinc deposition.

At low Reynolds numbers ($0.56 \leq Re_p \leq 5$), the single protrusion appears to redistribute the reaction instead of increasing the total mass flux to the electrode.⁴ That is, regions of enhanced mass transport appear to balance regions of diminished mass transport so that the the total mass flux is the same with or without the single protrusion. Aside from the mass transport enhancement immediately in front of the single protrusion (from convection toward the electrode—maximum flux at $y=-1.12 r_{cyl}$), mass transport is impeded

⁴Since numerical results were not obtained for higher Reynolds numbers, no conclusions are made about the total mass flux for $Re_p > 5$.

over a large area around the protrusion because of attenuated shear stresses at the electrode surface. The dimensionless current relaxes to unity at about $y = -5 r_{\text{cyl}}$ upstream of the protrusion, at about $z = \pm 6 r_{\text{cyl}}$ to either side of the protrusion, and at some $y > 10 r_{\text{cyl}}$ downstream of the protrusion. The FIDAP measurement domain was not large enough to determine the extent of the downstream effect. However, the dimensionless current probably exceeds unity for all Re_p between 0.56 and 5 over a region that is far enough downstream of the protrusion, as suggested by the dimensionless currents that exceeded unity near the downstream end of the FIDAP domain at $\text{Re}_p = 0.56, 1$, and 5. Downstream mass-transport enhancement makes intuitive sense because mass transport was inhibited over the FIDAP domain as indicated by the total dimensionless currents, which were slightly less than 1 (Table 4.7). In other words, the ions that could not react owing to presence of the protrusion react farther downstream instead, increasing the local dimensionless current above unity.

At low Reynolds numbers, an electrically conducting protrusion (such as a zinc nodule) is also expected to redistribute reactions instead of increasing the total mass flux. To a conducting protrusion itself, the total dimensionless current⁵ is expected to be greater than unity because the dimensionless shear stress would be greater than unity over large fractions of the protrusion (for cylindrical protrusions, for example, see Figure 2.17). In the wake of the protrusion, the dimensionless current would be less than unity because of depletion effects. This assertion is supported by the work of Rogers and Taylor [10]. From autoradiographs, they determined that mass transport of coumarin labeled with carbon-14 was enhanced to protrusions but attenuated in the wakes.

If striations do not form as a result of enhanced mass transport of zinc in the wake of zinc nuclei, then what is the mechanism for striation formation? Contaminants present in low concentrations should be considered as a possible cause. The results from this study indicate that contaminants would be preferentially deposited in front of zinc nuclei,

⁵To make it dimensionless, the total current to the conducting protrusion would be normalized by the background current to the electrode area underneath the protrusion.

where they would inhibit zinc deposition, making zinc deposition behind the nuclei the most favorable. This suggestion is attractive because mass-transport effects are more pronounced with minor species because they are more subject to depletion effects.⁶ Also, striations suddenly appear in copper or silver deposition when small quantities of contaminants (or additives) are purposely added to the electrolyte [16–18]. However, the literature results do not support this mechanism for zinc. Although zinc striations appear more rapidly in the presence of lead ion contamination (for example), zinc striations also appear in ultrapure zinc solutions [1]. However, it is possible that low levels of hydrogen assume the role of a contaminant for zinc. Hydrogen is present at low levels during zinc deposition even in ultrapure solutions because the open-circuit potential of zinc is -0.763 V.

An alternate explanation stems from the numerical and experimental results from the literature (see below) which suggest that zinc deposition rates can increase with decreasing zinc ion concentration (negative reaction orders). If this is the case, then higher deposition rates of zinc in the wake of nuclei may occur as a result of a depletion effect. Negative reaction orders are possible with S-shaped polarization kinetics. Such polarization curves have been observed by a number of investigators [17, 23–25] and have been numerically calculated by Lee and Jorné [26] using a kinetic mechanism similar to that of Epelboin *et al.* [23]. Figure 4.31, from Lee and Jorné [26], illustrates how lower zinc-ion concentrations may result in higher consumption rates of zinc from S-shaped kinetics. In the region of negative polarization resistance (where the slope of the consumption rate *vs.* potential curve is negative), the consumption rate is higher for $[Zn]=0.95$ than for $[Zn]=1$.

Zinc striations occur under conditions where negative polarization resistances are observed indicating that S-shaped kinetics may be responsible for striation formation. Copper striations that appear in the presence of additives are also accompanied by negative polarization resistances [21]. However, zinc striations also occur at current densities which are higher than the current densities at which negative polarization resistances are ob-

⁶Since zinc striations appear at low fractions of the limiting current, the concentration of zinc ions near the surface is not much different from the concentration of zinc ions in the bulk electrolyte.

Figure 4.31: The concentration dependence of S-shaped zinc kinetics on the consumption rate of zinc, taken from Lee and Jorné [26].

served [17]. A possible explanation for this may lie with the heterogeneous nature of the electrode surface. For example, Sutija [5, page 97] suggested an exchange current density for the zinc reaction of 100 mA/cm^2 on the nucleated growth centers and 1 mA/cm^2 on the surrounding electrode surface. The surrounding surface could be in the negative polarization regime while the nuclei themselves are well outside of it. However, Sutija [5] also suggested that the S-shaped polarization curves of Epelboin could be experimental artifacts because the current densities do not account for increasing surface area from the rough zinc deposit and because small errors in subtracting ohmic drop could produce a spurious backward-bending region of the curve.

There is still no completely satisfactory explanation for the formation of zinc striations. In future work, it would be interesting to deposit zinc within an array of $50 \text{ }\mu\text{m}$ tall insulating cylinders to determine whether the zinc would deposit preferentially in the wake region. Cylinders of this height would remain the dominant fluid-flow disturbance as zinc nuclei, $10 \text{ }\mu\text{m}$ in height or less, begin to meld into striations. The photosensitive polyimide used in this study provides a relatively easy method to produce the cylinders. As a result, several different protrusions arrays could be employed.

Appendix A

Supplementary Information on the Boundary-Integral Technique

A.1 The Lorentz reciprocal identity

The Lorentz reciprocal identity (equation 2.1, see also [29]) is used as the starting point for deriving the boundary-integral equations in Chapter 2. The identity can be derived using three equations: the Navier-Stokes equation for creeping flow; the definition of the stress tensor for a Newtonian fluid, σ_{ij} ; and the continuity equation. The indices ij run through the Cartesian coordinates (x,y,z) and a repeated subscript implies summation over this range. These three equations are

$$\frac{\partial \sigma_{ij}}{\partial x_j} = 0 = -\frac{\partial p}{\partial x_j} \delta_{ij} + \mu \frac{\partial^2 u_i}{\partial x_j^2} \quad (\text{A.1})$$

$$\sigma_{ij} = -p \delta_{ij} + \mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \quad (\text{A.2})$$

$$\frac{\partial u_j}{\partial x_j} = 0. \quad (\text{A.3})$$

δ_{ij} is equal to unity when $i = j$ and to zero when $i \neq j$. Equation A.1 is valid as long as the flow is regular (*i.e.*, the fluid velocity does not go to infinity at any point), as will be assumed in the remainder of this section of the appendix.

First, the double dot product is taken between equation A.2 and the tensor $(\partial u'_i/\partial x_j)$ to give the scalar relation

$$\sigma_{ij} \frac{\partial u'_i}{\partial x_j} = -p \delta_{ij} \frac{\partial u'_i}{\partial x_j} + \mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \frac{\partial u'_i}{\partial x_j}. \quad (\text{A.4})$$

The prime indicates that the flow u'_i is different from u_i . Since δ_{ij} is nonzero only when $i = j$, $\delta_{ij}(\partial u'_i/\partial x_j) = \partial u'_j/\partial x_j$, which is equal to zero from equation A.3. Hence, the pressure term drops from equation A.4 giving

$$\sigma_{ij} \frac{\partial u'_i}{\partial x_j} = \mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \frac{\partial u'_i}{\partial x_j}. \quad (\text{A.5})$$

The left side of equation A.5 can be written as

$$\sigma_{ij} \frac{\partial u'_i}{\partial x_j} = \frac{\partial}{\partial x_j} (\sigma_{ij} u'_i) - u'_i \frac{\partial \sigma_{ij}}{\partial x_j}. \quad (\text{A.6})$$

The right-most term in equation A.6 is zero because $(\partial \sigma_{ij}/\partial x_j) = 0$ from equation A.1. Equation A.6 then simplifies to

$$\sigma_{ij} \frac{\partial u'_i}{\partial x_j} = \frac{\partial}{\partial x_j} (\sigma_{ij} u'_i). \quad (\text{A.7})$$

Substituting equation A.7 into equation A.5 gives

$$\frac{\partial}{\partial x_j} (u'_i \sigma_{ij}) = \mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \frac{\partial u'_i}{\partial x_j}. \quad (\text{A.8})$$

Exchanging u_i for u'_i and σ_{ij} for σ'_{ij} in equation A.8 gives:

$$\frac{\partial}{\partial x_j} (u_i \sigma'_{ij}) = \mu \left(\frac{\partial u'_i}{\partial x_j} + \frac{\partial u'_j}{\partial x_i} \right) \frac{\partial u_i}{\partial x_j}. \quad (\text{A.9})$$

When equation A.9 is subtracted from equation A.8, two of the four terms on the right cancel yielding

$$\frac{\partial}{\partial x_j} (u'_i \sigma_{ij} - u_i \sigma'_{ij}) = \mu \left(\frac{\partial u_j}{\partial x_i} \frac{\partial u'_i}{\partial x_j} - \frac{\partial u'_j}{\partial x_i} \frac{\partial u_i}{\partial x_j} \right), \quad (\text{A.10})$$

and when the right side of equation A.10 is expanded, it becomes apparent that the sum of the remaining two terms is also zero. We are left with the reciprocal identity,

$$\frac{\partial}{\partial x_j} (u'_i \sigma_{ij} - u_i \sigma'_{ij}) = 0. \quad (\text{A.11})$$

A.2 Deduction of the assumed forms for $u_i(\mathbf{x})$ and $f_i(\mathbf{x})$

The velocity and force terms can be written in the form

$$\begin{aligned} u_x(x, \sigma, \phi) &= \cos(\phi) \mathcal{U}_x(x, \sigma) \\ u_\sigma(x, \sigma, \phi) &= \cos(\phi) \mathcal{U}_\sigma(x, \sigma) \\ u_\phi(x, \sigma, \phi) &= -\sin(\phi) \mathcal{U}_\phi(x, \sigma) \end{aligned} \tag{A.12}$$

$$\begin{aligned} f_x(x, \sigma, \phi) &= \cos(\phi) \mathfrak{F}_x(x, \sigma) \\ f_\sigma(x, \sigma, \phi) &= \cos(\phi) \mathfrak{F}_\sigma(x, \sigma) \\ f_\phi(x, \sigma, \phi) &= -\sin(\phi) \mathfrak{F}_\phi(x, \sigma) \end{aligned} \tag{A.13}$$

for linear infinite shear flow over an axisymmetric protrusion. Note that (x, σ, ϕ) are cylindrical coordinates, and $\mathcal{U}_x$, $\mathcal{U}_\sigma$, $\mathcal{U}_\phi$, $\mathfrak{F}_x$, $\mathfrak{F}_\sigma$, and $\mathfrak{F}_\phi$ are functions of x and σ only. The form of these equations is not new (see, for example, [41]). However, it is useful to show how these equations are deduced.

One starts by examining the boundary conditions. In Cartesian coordinates, the velocity distribution far from the protrusion is given by

$$\begin{aligned} u_x^\infty &= 0 \\ u_y^\infty &= \kappa(x - x_w) \\ u_z^\infty &= 0 \end{aligned} \tag{A.14}$$

where the wall is the plane at $x = x_w$ and κ is the shear rate far from the protrusion. It follows from A.14 that the force at the wall far from the protrusion is

$$\begin{aligned} f_x^\infty &= -p \\ f_y^\infty &= \kappa\mu \\ f_z^\infty &= 0 \end{aligned} \tag{A.15}$$

where p is the pressure.

In cylindrical coordinates, A.14 becomes

$$\begin{aligned} u_x^\infty &= 0 \\ u_\sigma^\infty &= \cos(\phi) u_y^\infty \\ u_\phi^\infty &= -\sin(\phi) u_y^\infty \end{aligned} \quad (\text{A.16})$$

and A.15 becomes

$$\begin{aligned} f_x^\infty &= -p \\ f_\sigma^\infty &= \kappa\mu \cos(\phi) \\ f_\phi^\infty &= -\kappa\mu \sin(\phi) \end{aligned} \quad (\text{A.17})$$

For linear infinite shear flow, the pressure is constant. One can see that f_x^∞ in equation A.17 is not of the same form as f_x in equation A.13. To avoid this problem, the pressure is set to zero far from the protrusion. This results in no loss of generality since a constant pressure can be added to the final solution if necessary.

Based on the form of A.16, we assume that u_σ and u_ϕ have the form

$$\begin{aligned} u_\sigma &= \cos(\phi) \mathfrak{U}_\sigma \\ u_\phi &= -\sin(\phi) \mathfrak{U}_\phi \end{aligned} \quad (\text{A.18})$$

everywhere in the domain. The form for u_x then follows from the continuity equation in cylindrical coordinates

$$\begin{aligned} u_x &= \cos(\phi) \mathfrak{U}_x \\ \mathfrak{U}_x &= \int \frac{1}{\sigma} (\mathfrak{U}_\phi - \frac{\partial(\sigma \mathfrak{U}_\sigma)}{\partial \sigma}) dx \end{aligned} \quad (\text{A.19})$$

As required, $\mathfrak{U}_x$, is a function of x and σ only.

For equations A.18 and A.19 to be valid, they must be consistent with the Navier-Stokes equations. That is, the $\cos(\phi)$ and $\sin(\phi)$ terms must all cancel. After A.18 and A.19 are substituted into the Navier-Stokes equations in cylindrical coordinates, the forms for u_x , u_σ , and u_ϕ are consistent with the equations as long as the pressure has the form

$$p = \mathfrak{P} \cos(\phi) \quad (\text{A.20})$$

where $\mathfrak{P}$ is a function of x and σ only. Note that $\mathfrak{P}$ approaches zero at infinity. The Navier-Stokes equations reduce to

$$\frac{\partial \mathfrak{P}}{\partial x} = \mu \left[\frac{1}{\sigma} \frac{\partial}{\partial \sigma} \left(\sigma \frac{\partial u_x}{\partial \sigma} \right) - \frac{u_x}{\sigma^2} + \frac{\partial^2 u_x}{\partial x^2} \right] \quad (\text{A.21})$$

$$\frac{\partial \mathfrak{P}}{\partial \sigma} = \mu \left[\frac{\partial}{\partial \sigma} \left(\frac{1}{\sigma} \frac{\partial (\sigma u_\sigma)}{\partial \sigma} \right) - \frac{u_\sigma}{\sigma^2} + \frac{2u_\phi}{\sigma^2} + \frac{\partial^2 u_\sigma}{\partial x^2} \right] \quad (\text{A.22})$$

$$\mathfrak{P} = -\mu \sigma \left[-\frac{\partial}{\partial \sigma} \left(\frac{1}{\sigma} \frac{\partial (\sigma u_\phi)}{\partial \sigma} \right) + \frac{u_\phi}{\sigma^2} - \frac{2u_\sigma}{\sigma^2} - \frac{\partial^2 u_\phi}{\partial x^2} \right] \quad (\text{A.23})$$

The form for the force components (equations A.13) follows directly from the form for the velocity components. The force components anywhere on the surface of the protrusion or the wall can be found by taking the dot product between the stress tensor, $\vec{\vec{\sigma}}$, and the unit vector normal to the surface, $\vec{n}$, where the single arrow indicates a vector and the double arrow indicates a second order tensor. The stress tensor, $\vec{\vec{\sigma}}$, should not be confused with the radial coordinate, σ .

For an axisymmetric domain, the normal vector can be written as

$$\vec{n} = C_x \vec{i}_x + C_\sigma \vec{i}_\sigma \quad (\text{A.24})$$

where $\vec{i}_x$ and $\vec{i}_\sigma$ are unit vectors in the x and σ directions and C_σ and C_x are constants chosen so that the magnitude of $\vec{n}$ is equal to unity. The ϕ component for the normal vector is zero for an axisymmetric domain.

It follows that the dot product between $\vec{\sigma}$ and $\vec{n}$ can be written as

$$\begin{aligned}
 \vec{\sigma}_{xx} \cdot \vec{n} &= \sigma_{xx} \vec{i}_x \vec{i}_x \cdot (C_x \vec{i}_x + C_\sigma \vec{i}_\sigma) = \sigma_{xx} C_x \vec{i}_x \\
 \vec{\sigma}_{\sigma\sigma} \cdot \vec{n} &= \sigma_{\sigma\sigma} \vec{i}_\sigma \vec{i}_\sigma \cdot (C_x \vec{i}_x + C_\sigma \vec{i}_\sigma) = \sigma_{\sigma\sigma} C_\sigma \vec{i}_\sigma \\
 \vec{\sigma}_{\phi\phi} \cdot \vec{n} &= \sigma_{\phi\phi} \vec{i}_\phi \vec{i}_\phi \cdot (C_x \vec{i}_x + C_\sigma \vec{i}_\sigma) = 0 \\
 \vec{\sigma}_{x\sigma} \cdot \vec{n} &= \sigma_{x\sigma} \vec{i}_x \vec{i}_\sigma \cdot (C_x \vec{i}_x + C_\sigma \vec{i}_\sigma) = \sigma_{x\sigma} C_\sigma \vec{i}_x \\
 \vec{\sigma}_{\sigma x} \cdot \vec{n} &= \sigma_{\sigma x} \vec{i}_\sigma \vec{i}_x \cdot (C_x \vec{i}_x + C_\sigma \vec{i}_\sigma) = \sigma_{\sigma x} C_x \vec{i}_\sigma \\
 \vec{\sigma}_{x\phi} \cdot \vec{n} &= \sigma_{x\phi} \vec{i}_x \vec{i}_\phi \cdot (C_x \vec{i}_x + C_\sigma \vec{i}_\sigma) = 0 \\
 \vec{\sigma}_{\phi x} \cdot \vec{n} &= \sigma_{\phi x} \vec{i}_\phi \vec{i}_x \cdot (C_x \vec{i}_x + C_\sigma \vec{i}_\sigma) = \sigma_{\phi x} C_x \vec{i}_\phi \\
 \vec{\sigma}_{\sigma\phi} \cdot \vec{n} &= \sigma_{\sigma\phi} \vec{i}_\sigma \vec{i}_\phi \cdot (C_x \vec{i}_x + C_\sigma \vec{i}_\sigma) = 0 \\
 \vec{\sigma}_{\phi\sigma} \cdot \vec{n} &= \sigma_{\phi\sigma} \vec{i}_\phi \vec{i}_\sigma \cdot (C_x \vec{i}_x + C_\sigma \vec{i}_\sigma) = \sigma_{\phi\sigma} C_\sigma \vec{i}_\phi
 \end{aligned} \tag{A.25}$$

where the nonzero values of $\sigma_{\alpha\beta}$ (α and β run through the cylindrical coordinates (x, σ, ϕ)) are

$$\begin{aligned}
 \sigma_{xx} &= -p + 2\mu \frac{\partial u_x}{\partial x} \\
 \sigma_{\sigma\sigma} &= -p + 2\mu \frac{\partial u_\sigma}{\partial \sigma} \\
 \sigma_{x\sigma} &= \sigma_{\sigma x} = \mu \left[\frac{\partial u_x}{\partial \sigma} + \frac{\partial u_\sigma}{\partial x} \right] \\
 \sigma_{x\phi} &= \sigma_{\phi x} = \mu \left[\frac{\partial u_\phi}{\partial x} + \frac{1}{\sigma} \frac{\partial u_x}{\partial \phi} \right] \\
 \sigma_{\sigma\phi} &= \sigma_{\phi\sigma} = \mu \left[\sigma \frac{\partial}{\partial \sigma} \left(\frac{u_\phi}{\sigma} \right) + \frac{1}{\sigma} \frac{\partial u_\sigma}{\partial \phi} \right]
 \end{aligned} \tag{A.26}$$

Substituting A.12 into A.26 and then substituting the result into A.25 gives

$$\begin{aligned}
 \vec{\sigma}_{xx} \cdot \vec{n} &= \left(-\mathfrak{P} \cos(\phi) + 2\mu \cos(\phi) \frac{\partial \mathfrak{U}_x}{\partial x} \right) C_x \vec{i}_x \\
 \vec{\sigma}_{\sigma\sigma} \cdot \vec{n} &= \left(-\mathfrak{P} \cos(\phi) + 2\mu \cos(\phi) \frac{\partial \mathfrak{U}_\sigma}{\partial \sigma} \right) C_\sigma \vec{i}_\sigma \\
 \vec{\sigma}_{x\sigma} \cdot \vec{n} &= \left(\mu \frac{\partial \mathfrak{U}_x}{\partial \sigma} \cos(\phi) + \mu \frac{\partial \mathfrak{U}_\sigma}{\partial x} \cos(\phi) \right) (C_\sigma \vec{i}_x + C_x \vec{i}_\sigma) \\
 \vec{\sigma}_{x\phi} \cdot \vec{n} &= \left(-\mu \frac{\partial \mathfrak{U}_\phi}{\partial x} \sin(\phi) - \mu \frac{\mathfrak{U}_x}{\sigma} \sin(\phi) \right) C_x \vec{i}_\phi \\
 \vec{\sigma}_{\sigma\phi} \cdot \vec{n} &= \left(\mu \sin(\phi) \left(\frac{\mathfrak{U}_\phi}{\sigma} - \frac{\partial \mathfrak{U}_\phi}{\partial \sigma} \right) - \mu \frac{\mathfrak{U}_\sigma}{\sigma} \sin(\phi) \right) C_\sigma \vec{i}_\phi
 \end{aligned} \tag{A.27}$$

Collecting the terms with common unit vectors and noting that $\mathcal{U}_x = \mathcal{U}_\sigma = \mathcal{U}_\phi = 0$ on the surface of the protrusion and wall yields

$$\begin{aligned}\vec{f}_x &= \vec{\sigma}_{xx} \cdot \vec{n} + \vec{\sigma}_{\sigma x} \cdot \vec{n} \\ &= \cos(\phi) \left\{ \left[-\mathfrak{P} + 2\mu \frac{\partial \mathcal{U}_x}{\partial x} \right] C_x + \left[\mu \frac{\partial \mathcal{U}_x}{\partial \sigma} + \mu \frac{\partial \mathcal{U}_\sigma}{\partial x} \right] C_\sigma \right\} \vec{i}_x \\ &= \cos(\phi) \mathfrak{F}_x \vec{i}_x.\end{aligned}\quad (\text{A.28})$$

$$\begin{aligned}\vec{f}_\sigma &= \vec{\sigma}_{\sigma\sigma} \cdot \vec{n} + \vec{\sigma}_{x\sigma} \cdot \vec{n} \\ &= \cos(\phi) \left\{ \left[-\mathfrak{P} + 2\mu \frac{\partial \mathcal{U}_\sigma}{\partial \sigma} \right] C_\sigma + \left[\mu \frac{\partial \mathcal{U}_x}{\partial \sigma} + \mu \frac{\partial \mathcal{U}_\sigma}{\partial x} \right] C_x \right\} \vec{i}_\sigma \\ &= \cos(\phi) \mathfrak{F}_\sigma \vec{i}_\sigma\end{aligned}\quad (\text{A.29})$$

$$\begin{aligned}\vec{f}_\phi &= \vec{\sigma}_{x\phi} \cdot \vec{n} + \vec{\sigma}_{\sigma\phi} \cdot \vec{n} \\ &= -\sin(\phi) \left\{ \mu \frac{\partial \mathcal{U}_\phi}{\partial \sigma} C_\sigma + \mu \frac{\partial \mathcal{U}_\phi}{\partial x} C_x \right\} \vec{i}_\phi \\ &= -\sin(\phi) \mathfrak{F}_\phi \vec{i}_\phi.\end{aligned}\quad (\text{A.30})$$

This verifies that the form for the force components given by A.13 is correct.

A.3 The shear stress and normal force at the surface

Equations for the wall shear stress, $\vec{\tau}_w$, the magnitude of the wall shear stress, $|\vec{\tau}_w|$, and the normal force on the wall, f_n , are presented here.

The wall shear stress, $\vec{\tau}_w$, is a vector quantity given by

$$\vec{\tau}_w = [(\vec{f}_x + \vec{f}_\sigma) \cdot \vec{t}] \vec{t} + \vec{f}_\phi. \quad (\text{A.31})$$

where $\vec{t}$ is a vector that is tangent to the surface pointing in the direction of increasing parametric distance S (see Figure 2.6). The tangent vector is given by

$$\vec{t} = -C_\sigma \vec{i}_x + C_x \vec{i}_\sigma \quad (\text{A.32})$$

where C_x and C_σ are the same constants used for defining the normal vector (equation A.24). $\vec{\tau}_w$ is plotted as a function of S in Figures 2.8 to 2.12 for several protrusion geometries in Chapter 2.

The magnitude of the shear stress, $|\tau_w|$, is

$$|\tau_w| = \sqrt{\left[(\vec{f}_x + \vec{f}_\sigma) \cdot \vec{t}\right]^2 + \vec{f}_\phi \cdot \vec{f}_\phi} \quad (\text{A.33})$$

The magnitude of the shear stress is used for the shear stress contours in Figures 2.15 to 2.16 in Chapter 2.

The normal force, f_n , is given by

$$\begin{aligned} f_n &= (\vec{f}_x + \vec{f}_\sigma) \cdot \vec{n} \\ &= -p = -\mathfrak{P} \cos(\phi). \end{aligned} \quad (\text{A.34})$$

f_n must be equal to $-p$, but this is not immediately obvious from equations A.28 and A.29.

A.4 Derivation of $f_n = -p = -\mathfrak{P} \cos(\phi)$

The normal force, f_n , on an axisymmetric surface is given by equation A.34. $\vec{f}_\phi$ does not appear in A.34 because it is tangent to all surfaces. Substituting the normal vector from A.24 and the forces from A.28 and A.29 into A.34, A.34 becomes

$$f_n = \cos(\phi) \left\{ \left[-\mathfrak{P} + 2\mu \frac{\partial \mathfrak{U}_x}{\partial x} \right] C_x^2 + \left[-\mathfrak{P} + 2\mu \frac{\partial \mathfrak{U}_\sigma}{\partial \sigma} \right] C_\sigma^2 + 2\mu C_x C_\sigma \left[\frac{\partial \mathfrak{U}_x}{\partial \sigma} + \frac{\partial \mathfrak{U}_\sigma}{\partial x} \right] \right\} \quad (\text{A.35})$$

Since $C_x^2 + C_\sigma^2 = 1$, the $\mathfrak{P}$ terms cancel giving

$$f_n = -\mathfrak{P} \cos(\phi) + 2\mu \cos(\phi) \left\{ \frac{\partial \mathfrak{U}_x}{\partial x} C_x^2 + \frac{\partial \mathfrak{U}_\sigma}{\partial \sigma} C_\sigma^2 + C_x C_\sigma \left[\frac{\partial \mathfrak{U}_x}{\partial \sigma} + \frac{\partial \mathfrak{U}_\sigma}{\partial x} \right] \right\} \quad (\text{A.36})$$

As shown below, the bracketed quantity $\{\}$ in equation A.36 is equal to zero for an arbitrary axisymmetric protrusion. The outline of an axisymmetric protrusion is shown in Figure A.1. In this figure, S is the parametric distance along the trace of the protrusion

Figure A.1: The trace of an axisymmetric protrusion in the $x\sigma$ plane. S is the parametric distance along the trace of the protrusion and the wall.

and the wall. With S defined in this fashion,

$$\frac{\partial \mathcal{U}_x}{\partial S} = \frac{\partial \mathcal{U}_\sigma}{\partial S} = 0 \quad (\text{A.37})$$

because $\mathcal{U}_x = \mathcal{U}_\sigma = 0$ everywhere on S . These derivatives can be written as

$$\begin{aligned} \frac{\partial \mathcal{U}_x}{\partial S} &= \left(\frac{\partial \mathcal{U}_x}{\partial x} \frac{\partial x}{\partial S} + \frac{\partial \mathcal{U}_x}{\partial \sigma} \frac{\partial \sigma}{\partial S} \right) = 0 \\ \frac{\partial \mathcal{U}_\sigma}{\partial S} &= \left(\frac{\partial \mathcal{U}_\sigma}{\partial x} \frac{\partial x}{\partial S} + \frac{\partial \mathcal{U}_\sigma}{\partial \sigma} \frac{\partial \sigma}{\partial S} \right) = 0 \end{aligned} \quad (\text{A.38})$$

From the tangent vector given by A.32, it follows that

$$\frac{\partial x}{\partial S} = -C_\sigma \quad \frac{\partial \sigma}{\partial S} = C_x \quad (\text{A.39})$$

Choosing the tangent vector is the same as choosing the direction of increasing S .

Substituting A.39 into A.38 gives

$$\begin{aligned} \left(-C_\sigma \frac{\partial \mathcal{U}_x}{\partial x} + C_x \frac{\partial \mathcal{U}_x}{\partial \sigma} \right) &= 0 \\ \left(-C_\sigma \frac{\partial \mathcal{U}_\sigma}{\partial x} + C_x \frac{\partial \mathcal{U}_\sigma}{\partial \sigma} \right) &= 0 \end{aligned} \quad (\text{A.40})$$

Multiplying the top equation in A.40 by C_σ and the bottom equation in A.40 by C_x gives

$$\begin{aligned} C_x C_\sigma \frac{\partial \mathcal{U}_x}{\partial \sigma} &= C_\sigma^2 \frac{\partial \mathcal{U}_x}{\partial x} \\ C_x C_\sigma \frac{\partial \mathcal{U}_\sigma}{\partial x} &= C_x^2 \frac{\partial \mathcal{U}_\sigma}{\partial \sigma} \end{aligned} \quad (\text{A.41})$$

When equation A.41 is substituted into A.36, the expression becomes

$$f_n = -\mathfrak{P} \cos(\phi) + 2\mu \cos(\phi) \left(\frac{\partial \mathfrak{U}_x}{\partial x} + \frac{\partial \mathfrak{U}_\sigma}{\partial \sigma} \right). \quad (\text{A.42})$$

The last term in A.42 is zero from continuity

$$\cos(\phi) \left(\frac{\mathfrak{U}_\sigma}{\sigma} + \frac{\partial \mathfrak{U}_\sigma}{\partial \sigma} + \frac{\partial \mathfrak{U}_x}{\partial x} - \frac{\mathfrak{U}_\phi}{\sigma} \right) = 0 \quad (\text{A.43})$$

because $\mathfrak{U}_\sigma = \mathfrak{U}_\phi = 0$ on the surface. Hence, equation A.42 reduces to

$$f_n = -p = -\mathfrak{P} \cos(\phi). \quad (\text{A.44})$$

$\mathfrak{P}$ is plotted in Figure A.2 for a cylindrical protrusion ($h/a=2$) and for a hemispherical protrusion. Plotting $\mathfrak{P}$ is equivalent to plotting the pressure distribution, p , on the downstream side of a protrusion ($\phi=0$).

A.5 The Green's functions in cylindrical coordinates

The Green's function in cylindrical coordinates, $N_{\alpha\beta}$, is related to the Green's function in Cartesian coordinates, G_{ij} , by equation 2.21. The free-space Green's function, G_{ij}^F , and the wall Green's function, G_{ij}^w , can be substituted for G_{ij} in equation 2.21. The corresponding Green's functions in cylindrical coordinates are designated by $N_{\alpha\beta}^F$ and $N_{\alpha\beta}^w$.

The free-space Green's function is given by

$$G_{ij}^F(\hat{\mathbf{x}}) = \frac{\delta_{ij}}{r} + \frac{\hat{x}_i \hat{x}_j}{r^3} \quad (\text{A.45})$$

$$r = |\hat{\mathbf{x}}| = \sqrt{\hat{x}^2 + \sigma^2 + \sigma_0^2 - 2\sigma\sigma_0 \cos(\hat{\phi})}.$$

Figure A.2: The function $\mathfrak{P}$ for a cylindrical protrusion ($h/a=2$) and a hemispherical protrusion as a function of the distance S (see Figure A.1). Plotting $\mathfrak{P}$ is equivalent to plotting the pressure distribution, p , on the downstream side of a protrusion ($\phi=0$) because $p = \mathfrak{P} \cos \phi$.

The $N_{\alpha\beta}^F$'s that correspond to $G_{ij}^F(\hat{\mathbf{x}})$ are

$$\begin{aligned}
 N_{xx}^F &= \frac{1}{r} + \frac{\hat{x}^2}{r^3} \\
 N_{x\sigma}^F &= \frac{\hat{x}}{r^3} [\sigma - \sigma_0 \cos(\hat{\phi})] \\
 N_{x\phi}^F &= \frac{\hat{x}\sigma_0}{r^3} \sin(\hat{\phi}) \\
 N_{\sigma x}^F &= \frac{\hat{x}}{r^3} [\sigma \cos(\hat{\phi}) - \sigma_0] \\
 N_{\sigma\sigma}^F &= \left(\frac{1}{r} + \frac{\sigma^2 + \sigma_0^2}{r^3} \right) \cos(\hat{\phi}) - \frac{\sigma\sigma_0}{r^3} (\cos^2(\hat{\phi}) + 1) \\
 N_{\sigma\phi}^F &= \left[- \left(\frac{1}{r} + \frac{\sigma_0^2}{r^3} \right) + \frac{\sigma\sigma_0}{r^3} \cos(\hat{\phi}) \right] \sin(\hat{\phi}) \\
 N_{\phi x}^F &= \frac{\hat{x}\sigma}{r^3} \sin(\hat{\phi}) \\
 N_{\phi\sigma}^F &= \left[\left(\frac{1}{r} + \frac{\sigma^2}{r^3} \right) - \frac{\sigma\sigma_0}{r^3} \cos(\hat{\phi}) \right] \sin(\hat{\phi}) \\
 N_{\phi\phi}^F &= \frac{1}{r} \cos(\hat{\phi}) + \frac{\sigma\sigma_0}{r^3} \sin^2(\hat{\phi})
 \end{aligned} \tag{A.46}$$

Except for a sign correction in the $N_{x\phi}$ term, these are identical to the $N_{\alpha\beta}$ terms in Pozrikidis [29, page 42].

The wall Green's function is zero at $x = x_w$. Namely,

$$G_{ij}^w(x = x_w, y, z) = 0. \tag{A.47}$$

Blake [69] divided the wall Green's function into a linear combination of two free-space Green's functions (G_{ij}^F), a potential dipole (G_{ij}^D), and a Stokeslet doublet (G_{ij}^{SD}) (see Pozrikidis [29, Section 7.2] for the meaning of the latter 2 terms). The expression he obtained was

$$G_{ij}^w(\hat{\mathbf{x}}) = G_{ij}^F(\hat{\mathbf{x}}) - G_{ij}^F(\hat{\mathbf{X}}) + 2h_0^2 G_{ij}^D(\hat{\mathbf{X}}) - 2h_0 G_{ij}^{SD}(\hat{\mathbf{X}}) \tag{A.48}$$

where $\hat{\mathbf{x}} = \mathbf{x} - \mathbf{x}_0$, $\hat{\mathbf{X}} = \mathbf{x} - \mathbf{x}_0^{\text{IM}}$, $\mathbf{x}_0^{\text{IM}} = (2x_w - x_0, y_0, z_0)$, and $h_0 = x_0 - x_w$. The functions G_{ij}^D and G_{ij}^{SD} are given by

$$\begin{aligned}
 G_{ij}^D(\hat{\mathbf{X}}) &= \pm \left(\frac{\delta_{ij}}{R^3} - 3 \frac{\hat{X}_i \hat{X}_j}{R^5} \right) \\
 G_{ij}^{SD}(\hat{\mathbf{X}}) &= \hat{X}_1 G_{ij}^D(\hat{\mathbf{X}}) \pm \frac{\delta_{j1} \hat{X}_i - \delta_{i1} \hat{X}_j}{R^3}
 \end{aligned} \tag{A.49}$$

with a minus sign for $j = 1$ corresponding to the x direction and a plus sign for $j = 2, 3$ for the y and z directions and where $R = |\hat{\mathbf{X}}| = \sqrt{\hat{X}_1^2 + \sigma^2 + \sigma_0^2 - 2\sigma\sigma_0\cos(\hat{\phi})}$. In the remainder of this section the subscript on $\hat{X}_1$ is dropped, and $\hat{X}_2$ and $\hat{X}_3$ are written as $\hat{y}$ and $\hat{z}$. That is,

$$\begin{aligned}\hat{X}_1 &= x - (2x_w - x_0) = \hat{X} \\ \hat{X}_2 &= \hat{y} \\ \hat{X}_3 &= \hat{z}\end{aligned}\tag{A.50}$$

In expanded form, the wall Green's function is

$$\begin{aligned}G_{11}^w &= G_{xx}^w = \left(\frac{1}{r} + \frac{\hat{x}^2}{r^3}\right) - \left(\frac{1}{R} + \frac{\hat{X}^2}{R^3}\right) - \frac{2h_0^2}{R^3} + \frac{6h_0^2\hat{X}^2}{R^5} + \frac{2h_0\hat{X}}{R^3} - \frac{6h_0\hat{X}^3}{R^5} \\ G_{12}^w &= G_{xy}^w = \frac{\hat{y}\hat{x}}{r^3} - \frac{\hat{y}\hat{X}}{R^3} - \frac{6h_0^2\hat{y}\hat{X}}{R^5} + \frac{6h_0\hat{y}\hat{X}^2}{R^5} + \frac{2h_0\hat{y}}{R^3} \\ G_{13}^w &= G_{xz}^w = \frac{\hat{z}\hat{x}}{r^3} - \frac{\hat{z}\hat{X}}{R^3} - \frac{6h_0^2\hat{z}\hat{X}}{R^5} + \frac{6h_0\hat{z}\hat{X}^2}{R^5} + \frac{2h_0\hat{z}}{R^3} \\ G_{21}^w &= G_{yx}^w = \frac{\hat{y}\hat{x}}{r^3} - \frac{\hat{y}\hat{X}}{R^3} + \frac{6h_0^2\hat{y}\hat{X}}{R^5} - \frac{6h_0\hat{y}\hat{X}^2}{R^5} + \frac{2h_0\hat{y}}{R^3} \\ G_{22}^w &= G_{yy}^w = \left(\frac{1}{r} + \frac{\hat{y}^2}{r^3}\right) - \left(\frac{1}{R} + \frac{\hat{y}^2}{R^3}\right) + \frac{2h_0^2}{R^3} - \frac{6h_0^2\hat{y}^2}{R^5} - \frac{2h_0\hat{X}}{R^3} + \frac{6h_0\hat{X}\hat{y}^2}{R^5} \tag{A.51} \\ G_{23}^w &= G_{yz}^w = G_{yz}^w = G_{zy}^w = \frac{\hat{z}\hat{y}}{r^3} - \frac{\hat{z}\hat{y}}{R^3} - \frac{6h_0^2\hat{z}\hat{y}}{R^5} + \frac{6h_0\hat{X}\hat{y}\hat{z}}{R^5} \\ G_{31}^w &= G_{zx}^w = \frac{\hat{z}\hat{x}}{r^3} - \frac{\hat{z}\hat{X}}{R^3} + \frac{6h_0^2\hat{z}\hat{X}}{R^5} - \frac{6h_0\hat{z}\hat{X}^2}{R^5} + \frac{2h_0\hat{z}}{R^3} \\ G_{33}^w &= G_{zz}^w = \left(\frac{1}{r} + \frac{\hat{z}^2}{r^3}\right) - \left(\frac{1}{R} + \frac{\hat{z}^2}{R^3}\right) + \frac{2h_0^2}{R^3} - \frac{6h_0^2\hat{z}^2}{R^5} - \frac{2h_0\hat{X}}{R^3} + \frac{6h_0\hat{X}\hat{z}^2}{R^5}\end{aligned}$$

The $N_{\alpha\beta}^w$ that correspond to the $G_{ij}^w(\hat{\mathbf{x}})$ are

$$\begin{aligned}
 N_{xx}^w &= G_{xx}^w \\
 N_{x\sigma}^w &= \left[\frac{\hat{x}}{r^3} - \frac{\hat{X}}{R^3} + \frac{6h_0^2\hat{X}}{R^5} - \frac{6h_0\hat{X}^2}{R^5} + \frac{2h_0}{R^3} \right] (\sigma - \sigma_0 \cos(\hat{\phi})) \\
 N_{x\phi}^w &= \left[\frac{\hat{x}}{r^3} - \frac{\hat{X}}{R^3} + \frac{6h_0^2\hat{X}}{R^5} - \frac{6h_0\hat{X}^2}{R^5} + \frac{2h_0}{R^3} \right] \sigma_0 \sin(\hat{\phi}) \\
 N_{\sigma x}^w &= \left[\frac{\hat{x}}{r^3} - \frac{\hat{X}}{R^3} - \frac{6h_0^2\hat{X}}{R^5} + \frac{6h_0\hat{X}^2}{R^5} + \frac{2h_0}{R^3} \right] (\sigma \cos(\hat{\phi}) - \sigma_0) \\
 N_{\sigma\sigma}^w &= \left(\frac{1}{r} + \frac{\sigma^2 + \sigma_0^2}{r^3} \right) \cos(\hat{\phi}) - \frac{\sigma\sigma_0}{r^3} (\cos^2(\hat{\phi}) + 1) \\
 &\quad - \left(\frac{1}{R} + \frac{\sigma^2 + \sigma_0^2}{R^3} \right) \cos(\hat{\phi}) + \frac{\sigma\sigma_0}{R^3} (\cos^2(\hat{\phi}) + 1) \\
 &\quad + \left[\frac{2h_0^2 - 2h_0\hat{X}}{R^3} + \frac{(6h_0\hat{X} - 6h_0^2)(\sigma^2 + \sigma_0^2)}{R^5} \right] \cos(\hat{\phi}) \\
 &\quad - \left[\frac{(6h_0\hat{X} - 6h_0^2)\sigma\sigma_0}{R^5} (\cos^2(\hat{\phi}) + 1) \right] \\
 N_{\sigma\phi}^w &= \left[- \left(\frac{1}{r} + \frac{\sigma_0^2}{r^3} \right) + \frac{\sigma\sigma_0}{r^3} \cos(\hat{\phi}) \right] \sin(\hat{\phi}) + \left[\left(\frac{1}{R} + \frac{\sigma_0^2}{R^3} \right) - \frac{\sigma\sigma_0}{R^3} \cos(\hat{\phi}) \right] \sin(\hat{\phi}) \\
 &\quad + \left\{ - \left[\frac{2h_0^2 - 2h_0\hat{X}}{R^3} + \frac{\sigma_0^2(6h_0\hat{X} - 6h_0^2)}{R^5} \right] + \left[\frac{\sigma\sigma_0(6h_0\hat{X} - 6h_0^2)}{R^5} \right] \cos(\hat{\phi}) \right\} \sin(\hat{\phi}) \\
 N_{\phi x}^w &= \left[\frac{\hat{x}}{r^3} - \frac{\hat{X}}{R^3} - \frac{6h_0^2\hat{X}}{R^5} + \frac{6h_0\hat{X}^2}{R^5} + \frac{2h_0}{R^3} \right] \sigma \sin(\hat{\phi}) \\
 N_{\phi\sigma}^w &= \left[\left(\frac{1}{r} + \frac{\sigma^2}{r^3} \right) - \frac{\sigma\sigma_0}{r^3} \cos(\hat{\phi}) \right] \sin(\hat{\phi}) - \left[\left(\frac{1}{R} + \frac{\sigma^2}{R^3} \right) - \frac{\sigma\sigma_0}{R^3} \cos(\hat{\phi}) \right] \sin(\hat{\phi}) \\
 &\quad + \left\{ \left[\frac{2h_0^2 - 2h_0\hat{X}}{R^3} + \frac{\sigma^2(6h_0\hat{X} - 6h_0^2)}{R^5} \right] - \frac{\sigma\sigma_0(6h_0\hat{X} - 6h_0^2)}{R^5} \cos(\hat{\phi}) \right\} \sin(\hat{\phi}) \\
 N_{\phi\phi}^w &= \frac{1}{r} \cos(\hat{\phi}) + \frac{\sigma\sigma_0}{r^3} \sin^2(\hat{\phi}) - \frac{1}{R} \cos(\hat{\phi}) - \frac{\sigma\sigma_0}{R^3} \sin^2(\hat{\phi}) \\
 &\quad + \frac{2h_0^2 - 2h_0\hat{X}}{R^3} \cos(\hat{\phi}) + \frac{\sigma\sigma_0(6h_0\hat{X} - 6h_0^2)}{R^5} \sin^2(\hat{\phi}).
 \end{aligned} \tag{A.52}$$

A.6 The calculation procedure for the integrals $Q_{\alpha\beta}$ and $Q'_{\alpha\beta}$

In Section 2.4, it was shown that the integrals over $\hat{\phi}$ could be written as

$$Q_{\alpha\beta}(\hat{x}(\hat{X}), \sigma, \sigma_0) = \int_0^{2\pi} N_{\alpha\beta}(\hat{x}(\hat{X}), \sigma, \sigma_0, \hat{\phi}) \cos(\hat{\phi}) d\hat{\phi} \quad (\text{A.53})$$

$$Q'_{\alpha\beta}(\hat{x}(\hat{X}), \sigma, \sigma_0) = \int_0^{2\pi} N_{\alpha\beta}(\hat{x}(\hat{X}), \sigma, \sigma_0, \hat{\phi}) \sin(\hat{\phi}) d\hat{\phi} \quad (\text{A.54})$$

where $\hat{X}$ is included for the wall Green's function.

For the free-space Green's function, $Q_{\alpha\beta}$ and $Q'_{\alpha\beta}$ can be written as a linear combination of the integrals I_{mn} given by

$$\begin{aligned} I_{mn}(\hat{x}, \sigma, \sigma_0) &\equiv \int_0^{2\pi} \frac{\cos^n(\omega)}{[\hat{x}^2 + \sigma^2 + \sigma_0^2 - 2\sigma\sigma_0 \cos(\omega)]^{m/2}} \\ &= \frac{4k^m}{(4\sigma\sigma_0)^{m/2}} \int_0^{\pi/2} \frac{(2\cos^2(\omega) - 1)^n}{(1 - k^2 \cos^2(\omega))^{m/2}} \end{aligned} \quad (\text{A.55})$$

where

$$k^2 = \frac{4\sigma\sigma_0}{(\sigma + \sigma_0)^2 + \hat{x}^2} \quad (\text{A.56})$$

For the wall Green's function, $Q_{\alpha\beta}$ and $Q'_{\alpha\beta}$ can be written as a linear combination of the integrals I_{mn} and I_{mn}^{IM} , where I_{mn}^{IM} is given by

$$\begin{aligned} I_{mn}^{\text{IM}}(\hat{X}, \sigma, \sigma_0) &\equiv \int_0^{2\pi} \frac{\cos^n(\omega)}{[\hat{X}^2 + \sigma^2 + \sigma_0^2 - 2\sigma\sigma_0 \cos(\omega)]^{m/2}} \\ &= \frac{4(k^{\text{IM}})^m}{(4\sigma\sigma_0)^{m/2}} \int_0^{\pi/2} \frac{(2\cos^2(\omega) - 1)^n}{(1 - (k^{\text{IM}})^2 \cos^2(\omega))^{m/2}} \end{aligned} \quad (\text{A.57})$$

and where

$$(k^{\text{IM}})^2 = \frac{4\sigma\sigma_0}{(\sigma + \sigma_0)^2 + \hat{X}^2} \quad (\text{A.58})$$

The only difference between I_{mn}^{IM} and I_{mn} is that k^{IM} replaces k and $\hat{X}$ replaces $\hat{x}$. The only difference between k^{IM} and k is that $\hat{X}$ replaces $\hat{x}$.

The $Q_{\alpha\beta}$ and $Q'_{\alpha\beta}$ for the free-space Green's function are given by

$$Q_{xx} = I_{11} + I_{31} \hat{x}^2$$

$$Q_{x\sigma} = (I_{31} \sigma - I_{32} \sigma_0) \hat{x}$$

$$Q'_{x\phi} = (I_{30} - I_{32}) \sigma_0 \hat{x}$$

$$Q_{\sigma x} = (I_{32} \sigma - I_{31} \sigma_0) \hat{x}$$

$$Q_{\sigma\sigma} = I_{12} - (I_{31} + I_{33}) \sigma \sigma_0 + I_{32} (\sigma^2 + \sigma_0^2)$$

$$Q'_{\sigma\phi} = -I_{10} + I_{12} + (I_{31} - I_{33}) \sigma \sigma_0 - (I_{30} - I_{32}) \sigma_0^2$$

$$Q'_{\phi x} = (I_{30} - I_{32}) \sigma \hat{x}$$

$$Q'_{\phi\sigma} = I_{10} - I_{12} + (I_{30} - I_{32}) \sigma^2 - (I_{31} - I_{33}) \sigma \sigma_0$$

$$Q_{\phi\phi} = I_{12} + (I_{31} - I_{33}) \sigma \sigma_0$$

The $Q_{\alpha\beta}$ and $Q'_{\alpha\beta}$ for the wall Green's function are given by

$$Q_{xx} = I_{11} - I_{11}^{\text{IM}} + I_{31} \hat{x}^2 - I_{31}^{\text{IM}} \hat{X}^2 - I_{31}^{\text{IM}} (2h_0^2 - 2h_0 \hat{X}) + 6I_{51}^{\text{IM}} (h_0^2 \hat{X}^2 - h_0 \hat{X}^3)$$

$$Q_{x\sigma} = (I_{31} \sigma - I_{32} \sigma_0) \hat{x} + (I_{31}^{\text{IM}} \sigma - I_{32}^{\text{IM}} \sigma_0) (2h_0 - \hat{X}) \\ + (I_{51}^{\text{IM}} \sigma - I_{52}^{\text{IM}} \sigma_0) (6h_0^2 \hat{X} - 6h_0 \hat{X}^2)$$

$$Q'_{x\phi} = (I_{30} - I_{32}) \sigma_0 \hat{x} - (I_{30}^{\text{IM}} - I_{32}^{\text{IM}}) (-2h_0 \sigma_0 + \sigma_0 \hat{X}) \\ + (I_{50}^{\text{IM}} - I_{52}^{\text{IM}}) (6h_0^2 \sigma_0 \hat{X} - 6h_0 \sigma_0 \hat{X}^2)$$

$$Q_{\sigma x} = (I_{32} \sigma - I_{31} \sigma_0) \hat{x} - (I_{32}^{\text{IM}} \sigma - I_{31}^{\text{IM}} \sigma_0) \hat{X} - 6h_0^2 (I_{52}^{\text{IM}} \sigma - I_{51}^{\text{IM}} \sigma_0) \hat{X} \\ + 2h_0 (I_{32}^{\text{IM}} \sigma - I_{31}^{\text{IM}} \sigma_0) + 6h_0 (I_{52}^{\text{IM}} \sigma - I_{51}^{\text{IM}} \sigma_0) \hat{X}^2$$

$$Q_{\sigma\sigma} = I_{12} - I_{12}^{\text{IM}} - (I_{31} + I_{33}) \sigma \sigma_0 + (I_{31}^{\text{IM}} + I_{33}^{\text{IM}}) \sigma \sigma_0 + I_{32} (\sigma^2 + \sigma_0^2) - I_{32}^{\text{IM}} (\sigma^2 + \sigma_0^2) \\ + I_{32}^{\text{IM}} (2h_0^2 - 2h_0 \hat{X}) + I_{52}^{\text{IM}} (\sigma^2 + \sigma_0^2) (-6h_0^2 + 6h_0 \hat{X}) \\ - (I_{51}^{\text{IM}} + I_{53}^{\text{IM}}) \sigma \sigma_0 (-6h_0^2 + 6h_0 \hat{X})$$

$$\begin{aligned}
Q'_{\sigma\phi} = & -I_{10} + I_{12} + I_{10}^{\text{IM}} - I_{12}^{\text{IM}} + (I_{31} - I_{33}) \sigma \sigma_0 - (I_{30} - I_{32}) \sigma_0^2 + (I_{30}^{\text{IM}} - I_{32}^{\text{IM}}) \sigma_0^2 \\
& - (I_{31}^{\text{IM}} - I_{33}^{\text{IM}}) \sigma \sigma_0 - I_{30}^{\text{IM}} (2h_0^2 - 2h_0 \hat{X}) + I_{32}^{\text{IM}} (2h_0^2 - 2h_0 \hat{X}) \\
& + (I_{51}^{\text{IM}} - I_{53}^{\text{IM}}) \sigma \sigma_0 (-6h_0^2 + 6h_0 \hat{X}) - (I_{50}^{\text{IM}} - I_{52}^{\text{IM}}) \sigma_0^2 (-6h_0^2 + 6h_0 \hat{X})
\end{aligned}$$

$$\begin{aligned}
Q'_{\phi x} = & (I_{30} - I_{32}) \sigma \hat{x} - (I_{30}^{\text{IM}} - I_{32}^{\text{IM}}) \sigma \hat{X} - 6h_0^2 (I_{50}^{\text{IM}} - I_{52}^{\text{IM}}) \sigma \hat{X} \\
& + 2h_0 (I_{30}^{\text{IM}} - I_{32}^{\text{IM}}) \sigma + 6h_0 (I_{50}^{\text{IM}} - I_{52}^{\text{IM}}) \sigma \hat{X}^2
\end{aligned}$$

$$\begin{aligned}
Q'_{\phi\sigma} = & I_{10} - I_{12} - I_{10}^{\text{IM}} + I_{12}^{\text{IM}} + (I_{30} - I_{32}) \sigma^2 - (I_{30}^{\text{IM}} - I_{32}^{\text{IM}}) \sigma^2 - (I_{31} - I_{33}) \sigma \sigma_0 \\
& + (I_{31}^{\text{IM}} - I_{33}^{\text{IM}}) \sigma \sigma_0 + (I_{30}^{\text{IM}} - I_{32}^{\text{IM}}) (2h_0^2 - 2h_0 \hat{X}) \\
& + (I_{50}^{\text{IM}} - I_{52}^{\text{IM}}) \sigma^2 (-6h_0^2 + 6h_0 \hat{X}) - (I_{51}^{\text{IM}} - I_{53}^{\text{IM}}) \sigma \sigma_0 (-6h_0^2 + 6h_0 \hat{X})
\end{aligned}$$

$$\begin{aligned}
Q_{\phi\phi} = & I_{12} - I_{12}^{\text{IM}} + (I_{31} - I_{33}) \sigma \sigma_0 - (I_{31}^{\text{IM}} - I_{33}^{\text{IM}}) \sigma \sigma_0 + I_{32}^{\text{IM}} (2h_0^2 - 2h_0 \hat{X}) \\
& + (I_{51}^{\text{IM}} - I_{53}^{\text{IM}}) \sigma \sigma_0 (-6h_0^2 + 6h_0 \hat{X})
\end{aligned}$$

The integrals I_{mn} and I_{mn}^{IM} can be written as linear combinations of the complete elliptic integrals of the first kind, E , and the second kind, F [70, Section 2.58], where E and F are given by

$$E(k) = \int_0^{\pi/2} \sqrt{1 - k^2 \cos^2(\omega)} d\omega \quad F(k) = \int_0^{\pi/2} \frac{d\omega}{\sqrt{1 - k^2 \cos^2(\omega)}} \quad (\text{A.67})$$

The elliptic integrals for I_{mn}^{IM} are identical to A.67 with k^{IM} in place of k . The symbols E^{IM} and F^{IM} are used for the elliptic integrals when k^{IM} is the parameter. In terms of E and F , the I_{mn} are given by

$$\begin{aligned}
I_{10} &= \frac{2 F k}{(\sigma \sigma_0)^{0.5}} \\
I_{11} &= \frac{2 k}{(\sigma \sigma_0)^{0.5}} \left(\frac{-2 E}{k^2} + \frac{F (2 - k^2)}{k^2} \right) \\
I_{12} &= \frac{2 (-8 E + 8 F + 4 E k^2 - 8 F k^2 + 3 F k^4)}{3 k^3 (\sigma \sigma_0)^{0.5}}
\end{aligned}$$

$$\begin{aligned}
I_{30} &= \frac{E k^3}{2 (1 - k^2) (\sigma \sigma_0)^{1.5}} \\
I_{31} &= \frac{k}{(\sigma \sigma_0)^{1.5}} \left(-F + \frac{E (2 - k^2)}{2 (1 - k^2)} \right) \\
I_{32} &= \frac{1}{2 (\sigma \sigma_0)^{1.5}} \left(\frac{F (-8 + 4 k^2)}{k} + \frac{E (4 - 4 k^2 + k^4 + 4 (1 - k^2))}{k (1 - k^2)} \right) \\
I_{33} &= \frac{k^3}{2 (\sigma \sigma_0)^{1.5}} \left(\frac{2 F (-32 + 32 k^2 - 9 k^4)}{3 k^6} + \frac{E (-64 + 96 k^2 - 38 k^4 + 3 k^6)}{3 k^6 (-1 + k^2)} \right) \\
I_{50} &= \frac{k^5}{8 (\sigma \sigma_0)^{2.5}} \left(\frac{-F}{3 (1 - k^2)} + \frac{2 E (2 - k^2)}{3 (1 - k^2)^2} \right) \\
I_{51} &= \frac{k^5}{8 (\sigma \sigma_0)^{2.5}} \left(\frac{F (-2 + k^2)}{3 k^2 (1 - k^2)} + \frac{E (2 - 2 k^2 (1 - k^2))}{3 k^2 (1 - k^2)^2} \right) \\
I_{52} &= \frac{k^5}{8 (\sigma \sigma_0)^{2.5}} \left(\frac{F (8 - 8 k^2 - k^4)}{3 k^4 (1 - k^2)} + \frac{E (-8 + 12 k^2 - 2 k^6)}{3 k^4 (1 - k^2)^2} \right) \\
I_{53} &= \left(\frac{1}{24 k (-1 + k^2)^2 (\sigma \sigma_0)^{2.5}} \right) (-64 E + 64 F + 128 E k^2 - 160 F k^2 - 66 E k^4 \\
&\quad + 126 F k^4 + 2 E k^6 - 29 F k^6 + 2 E k^8 - F k^8)
\end{aligned}$$

I_{mn}^{im} is identical to I_{mn} with E^{im} , F^{im} , and k^{im} in place of E , F , and k .

One procedure for efficiently calculating F and E [71, p.139] is:

$$F = \frac{\pi}{2} (1 + K_1)(1 + K_2)(1 + K_3) \cdots \quad E = F \left(1 - \frac{k^2}{2} P \right) \quad (\text{A.69})$$

where

$$K_0 = k \quad K_p = \frac{1 - C}{1 + C} \quad C = \sqrt{1 - K_{p-1}^2} \quad (\text{A.70})$$

and

$$P = 1 + \frac{K_1}{2} \left(1 + \frac{K_2}{2} \left(1 + \frac{K_3}{2} (\cdots) \cdots \right) \right) \quad (\text{A.71})$$

As verified below, F tends toward infinity as $-\ln(|\hat{\mathbf{x}}|)$ and E tends toward unity in the vicinity of the pole, $\mathbf{x}_0$. Taking the limit $\mathbf{x} \rightarrow \mathbf{x}_0$ of the functions $Q_{\alpha\beta}$ and I_{mn} that were

given above ($k \rightarrow 1$, $\sigma \rightarrow \sigma_0$, $x \rightarrow x_0$, $F \approx \ln(|\hat{\mathbf{x}}|)$, $E \approx 1$), it becomes apparent that Q_{xx} , $Q_{\sigma\sigma}$, and $Q_{\phi\phi}$ tend toward infinity as $-2\ln(|\hat{\mathbf{x}}|)$, $-2\ln(|\hat{\mathbf{x}}|)$, and $-4\ln(|\hat{\mathbf{x}}|)$, respectively, and that the other $Q_{\alpha\beta}$ tend toward constant values. This is true for both the free-space Green's function and the wall Green's function.

To verify the asymptotic behavior of F and E in the vicinity of the pole, it is easiest to examine the polynomial expansions for F and E provided by Abramowitz and Stegun [35, Section 17]:

$$\begin{aligned}
 F &= [a_0 + a_1 m_1 + a_2 m_1^2] + [b_0 + b_1 m_1 + b_2 m_1^2] \ln(1/m_1) \\
 a_0 &= \ln(4) & b_0 &= 0.5 \\
 a_1 &= 0.1119723 & b_1 &= 0.1213478 \\
 a_2 &= 0.0725296 & b_2 &= 0.0288729
 \end{aligned} \tag{A.72}$$

$$\begin{aligned}
 E &= [1 + a_1 m_1 + a_2 m_1^2] + [b_1 m_1 + b_2 m_1^2] \ln(1/m_1) \\
 a_1 &= 0.4630151 & b_1 &= 0.2452727 \\
 a_2 &= 0.1077812 & b_2 &= 0.0412496
 \end{aligned} \tag{A.73}$$

where $m_1 = (1 - k^2)$. As the pole is approached $m_1 \rightarrow 0$ and

$$\begin{aligned}
 F &\approx 0.5 \ln \left(\frac{1}{1 - k^2} \right) + \ln(4) \\
 E &\approx 1
 \end{aligned} \tag{A.74}$$

It can be shown that F increases toward infinity at the same rate as

$$\lim_{\hat{\mathbf{x}} \rightarrow \mathbf{x}_0} -\ln(|\hat{\mathbf{x}}|) \tag{A.75}$$

by showing that the limit

$$\lim_{\hat{\mathbf{x}} \rightarrow \mathbf{x}_0} \left(\ln \left[\frac{4}{(1 - k^2)^{0.5}} \right] + \ln(|\hat{\mathbf{x}}|) \right) \tag{A.76}$$

is a constant. The constant happens to be $\ln(8\sigma_0)$.

A.7 Demonstration that the disturbance force decreases as $1/r^3$ far from the protrusion

For the force balance in Section 2.11, the integral of the disturbance force over a surface D_i far from the protrusion was required to be zero. Specifically, it was required that

$$\int_{D_i} \sigma_{ik}^p n_k dS = \int_{D_i} f_i^p(\mathbf{x}) dS = 0. \quad (\text{A.77})$$

where $f_i^p(\mathbf{x}) = \sigma_{ik}^p(\mathbf{x}) n_k$ and the surface D_i is shown in Figure 2.2. For equation A.77 to be valid, $f_i^p(\mathbf{x})$ must decrease faster than $1/r^2$ because the area of the surface at infinity increases as r^2 . For flow around a sphere in an infinite medium, $f_i^p(\mathbf{x})$ decreases as $1/r^2$, and the integral of the disturbance force at infinity approaches a constant instead of zero. For a protrusion on a wall, however, the disturbance force decreases as $1/r^3$, as shown below.

Blake [69] showed that the disturbance in the stress tensor decreases as $1/r^3$ for a point force g_i above a plane wall. If the integral equation for a protrusion on a plane wall (equation 2.13) is simply an integral of point forces in the vicinity of a wall, then $f_i^p(\mathbf{x})$ in equation A.77 also decreases as $1/r^3$ because of the linearity of the creeping flow equations.

The equation for the velocity due to a point force g_i in the vicinity of a plane wall is

$$u_j(\mathbf{x}_0) = \frac{1}{8\pi\mu} G_{ij}^w(\mathbf{x}, \mathbf{x}_0) g_i, \quad (\text{A.78})$$

where G_{ij}^w is the wall Green's function. If g_i is assumed to be infinitesimal, then it can be replaced by $f_i(\mathbf{x}) dS$ and equation A.78 becomes

$$d[u_j(\mathbf{x}_0)] = \frac{1}{8\pi\mu} G_{ij}^w(\mathbf{x}, \mathbf{x}_0) f_i(\mathbf{x}) dS. \quad (\text{A.79})$$

Integrating equation A.79 over some surface D_p yields

$$u_j(\mathbf{x}_0) = \frac{1}{8\pi\mu} \int_{D_p} G_{ij}^w(\mathbf{x}, \mathbf{x}_0) f_i(\mathbf{x}) dS + \text{constant} \quad (\text{A.80})$$

where the constant is zero because u_j is zero when $S = 0$. Equation A.80 is identical in form to equation 2.13.

When the wall Green's function is used in equation 2.13, it reduces to

$$-u_j^p(\mathbf{x}_0) = \frac{1}{8\pi\mu} \int_{D_p} G_{ij}^w(\hat{\mathbf{x}}, \mathbf{x}_0) f_i(\mathbf{x}) dS(\mathbf{x}), \quad (\text{A.81})$$

where the integral is over the surface of the protrusion, D_p , only. By comparing equations A.81 and equations A.80, it is apparent that $-u_j^p$ is the disturbance velocity resulting from a distributed force per unit area in the vicinity of a plane wall. Hence, $f_i^p(\mathbf{x})$ decreases as $1/r^3$.

A.8 Comparison of the numerical results to exact solutions

To test the numerical accuracy of our boundary-integral code, the numerical calculations were compared to calculations based on "exact" formulations from the literature. Our boundary-integral formulation cannot be considered exact because the force was approximated as a constant over each element (Section 2.5). As a result of this numerical testing, we can be confident in our numerical result to at least three significant digits. The literature results that were used for comparison all involve three-dimensional flow around either axisymmetric protrusions on a plane wall or axisymmetric obstacles above a plane wall. As long as the wall Green's function is used, our boundary-integral code can be used to treat axisymmetric obstacles above a plane wall. With some alterations to the code, the free-space Green's function could also have been used.

For an obstacle above a plane wall, the goal of most of the literature calculations was to determine the total force and torque on the obstacle by the fluid. Goldman, Cox, and Brenner [33] calculated these quantities for a fixed sphere in the vicinity of a plane wall, and O'Neill [30] calculated these quantities for a sphere touching a plane wall. Price [31] treated the problem of a hemispherical protrusion on a plane wall. He calculated the total force and torque acting on the protrusion. He also determined the position of two points where the shear stress was zero in the xy plane (see Figure 2.3 for the coordinate system). These points of zero shear stress are shown in Figure A.3. The first point is on the

Figure A.3: The points of zero shear stress on a hemispherical protrusion. The angle θ_0 is defined.

hemisphere at $\theta_0 = 73.2^\circ$ (see Figure A.3), and the other point is on the wall at $y/R = 1.22$, where R is the radius of the hemisphere.

Before comparing our results to the literature, our calculation procedures are described for the total force, the total torque, and the points of zero shear stress. For axisymmetric geometries, the only non-zero component of the total force is in the y -direction, and the only nonzero component of the total torque is in the z -direction. For a positive torque in the z -direction, a sphere (that is allowed to rotate about its center) will rotate so that the surface of the sphere closest to the wall moves in the negative y direction.

To calculate the total force, the force is expressed in Cartesian coordinates by substituting equation 2.16 into equation 2.17 to give

$$\begin{aligned}
 f_x \vec{i}_x &= \mathfrak{F}_x \cos(\phi) \vec{i}_x \\
 f_y \vec{i}_y &= (\mathfrak{F}_\sigma \cos^2(\phi) + \mathfrak{F}_\phi \sin^2(\phi)) \vec{i}_y \\
 f_z \vec{i}_z &= (\mathfrak{F}_\sigma \cos(\phi) \sin(\phi) - \mathfrak{F}_\phi \cos(\phi) \sin(\phi)) \vec{i}_z
 \end{aligned}
 \tag{A.82}$$

where $\vec{f} = f_x \vec{i}_x + f_y \vec{i}_y + f_z \vec{i}_z$ and $\vec{i}_x$, $\vec{i}_y$, and $\vec{i}_z$ are unit vectors.

The total force in the y-direction, F_y , for any arbitrary axisymmetric protrusion is

$$F_y = \int \vec{f} \cdot \vec{i}_y dS = \int_0^l \int_0^{2\pi} (\mathfrak{F}_\sigma \cos^2(\phi) + \mathfrak{F}_\phi \sin^2(\phi)) \sigma d\phi dl \quad (\text{A.83})$$

where l is the length of the curve that coincides with the outline of the protrusion in the xy plane. Since $\mathfrak{F}_\sigma$ and $\mathfrak{F}_\phi$ are independent of ϕ , the integrals in the ϕ direction can be evaluated to give

$$F_y = \pi \int_0^l \mathfrak{F}_\sigma \sigma dl + \pi \int_0^l \mathfrak{F}_\phi \sigma dl. \quad (\text{A.84})$$

For a sphere or a hemisphere, $dl = R|d\psi| = R d\psi$, where the ψ coordinate is shown in Figure A.4. The absolute value sign is not needed if one is careful to take the integral in the positive ψ direction. Substituting $dl = R d\psi$ and $\sigma = R \sin(\psi)$ into equation A.84 gives

$$F_y = \pi R^2 \int_0^{\psi_{N+1}} \mathfrak{F}_\sigma \sin(\psi) d\psi + \pi R^2 \int_0^{\psi_{N+1}} \mathfrak{F}_\phi \sin(\psi) d\psi \quad (\text{A.85})$$

where ψ_{N+1} is the total angle subtended by the protrusion. Since $\mathfrak{F}_\sigma$ and $\mathfrak{F}_\phi$ were assumed to be constant over each element (Section 2.5), the integrals over ψ can be evaluated over each element separately. Hence the total force on the protrusion is

$$F_y = -\pi R^2 \sum_{i=1}^N (\mathfrak{F}_{\sigma i} + \mathfrak{F}_{\phi i}) (\cos(\psi_{i+1}) - \cos(\psi_i)) \quad (\text{A.86})$$

where N is the total number of elements on the sphere or hemisphere.

For axisymmetric geometries, the total torque about the center of the sphere or hemisphere is equal to the z-component of the torque, T_z , which is given by

$$T_z \vec{i}_z = \int \vec{r}_c \times \vec{f} dS \quad (\text{A.87})$$

where $\vec{r}_c = (x - x_c) \vec{i}_x + \sigma \cos(\phi) \vec{i}_y + \sigma \sin(\phi) \vec{i}_z$ and x_c is the x-location of the center of the sphere or hemisphere. The r_c coordinate is shown in Figure A.4. Taking the cross product $\vec{r}_c \times \vec{f}$ (using equation A.82 for the force) and keeping only the nonzero integrals gives

$$T_z = \int_0^l \int_0^{2\pi} [-\sigma \mathfrak{F}_x + (x - x_c) \mathfrak{F}_\sigma] \cos^2(\phi) \sigma d\phi dl + \int_0^l \int_0^{2\pi} (x - x_c) \mathfrak{F}_\phi \sin^2(\phi) \sigma d\phi dl. \quad (\text{A.88})$$

Figure A.4: A schematic showing the ψ and r_c coordinates. The ψ and r_c coordinates are the same as the θ and r coordinates except they are translated a distance x_c from the origin along the x axis.

Substituting $dl = R d\psi$, $\sigma = R \sin(\psi)$, and $(x - x_c) = R \cos(\psi)$ into equation A.84, evaluating the integrals over ϕ , and evaluating the integrals over dl over each element separately gives

$$T_z = \pi R^3 \sum_i^N \left\{ -\frac{\mathfrak{F}_{xi}}{4} [2(\psi_{i+1} - \psi_i) - \sin(2\psi_{i+1}) + \sin(2\psi_i)] + \frac{1}{2} (\mathfrak{F}_{\sigma i} + \mathfrak{F}_{\phi i}) [-\cos^2(\psi_{i+1}) + \cos^2(\psi_i)] \right\}. \quad (\text{A.89})$$

To calculate the points of zero shear stress in the xy plane, the wall shear stress, τ_w , is written as

$$\tau_w \vec{t} = [(\vec{f}_x + \vec{f}_\sigma) \cdot \vec{t}] \vec{t} \quad (\text{A.90})$$

where the tangent vector, $\vec{t}$, points in the direction of increasing parametric arc length S (S is defined in Figure 2.6). Equation A.31 reduces to equation A.90 in the xy plane because f_ϕ is zero in the xy plane. The points of zero shear stress are determined by linear interpolation between the nodes where the shear stress changes sign.

Next, our calculations are compared to the literature calculations for a hemispherical protrusion, using both the free-space Green's function and the wall Green's function. When the free-space Green's function is used, the hemisphere, the wall, and the wall under the hemisphere need to be discretized (or meshed—see Figure 2.4). For the free-space Green's function, the following ratios were chosen for the dimensions of the mesh and the number of elements on the mesh

$$L_{\text{hemi}} : L_{\text{wall}} : L_{\text{under}} = \pi : 4\pi : 1$$

$$N_{\text{hemi}} : N_{\text{wall}} : N_{\text{under}} = 2 : 4 : 1$$

where L_{hemi} , L_{wall} , and L_{under} are the lengths of the mesh on the hemisphere, on the wall, and under the hemisphere, respectively, and N_{hemi} , N_{wall} , and N_{under} are the number of elements on the hemisphere, on the wall, and under the hemisphere, respectively. The total number of nodes (or collocation points) is equal to $N_{\text{hemi}} + N_{\text{wall}}$ because the elements under the hemisphere do not increase the size of the matrix to be solved. The size of each

Table A.1: The convergence of the dimensionless force, the dimensionless torque, and the locations of the points of zero shear stress to the literature values from Price [31] for a hemispherical protrusion. Our numerical calculations in this table were done with the free-space Green's function.

Free-space Green's function - hemispherical protrusion				
$N_{\text{hemi}}, N_{\text{wall}}, N_{\text{under}}$	Total dimensionless force on hemisphere $\frac{F_y}{\kappa\mu\pi R^2}$	Total dimensionless torque on hemisphere $\frac{T_z}{\kappa\mu\pi R^3}$	Angle on hemisphere where $\tau_w = 0$ (degrees)	Position on wall (y/R) where $\tau_w = 0$
4, 8, 2	4.27	2.38	75.1	1.14
6, 12, 3	4.28	2.42	76.5	1.20
8, 16, 4	4.29	2.43	73.0	1.22
10, 20, 5	4.29	2.43	74.1	1.20
12, 24, 6	4.29	2.44	74.1	1.18
16, 32, 8	4.29	2.44	73.7	1.18
20, 40, 10	4.30	2.44	73.4	1.21
26, 52, 13	4.30	2.44	73.4	1.21
32, 64, 16	4.30	2.44	73.3	1.21
Price [31]	4.30	2.44	73.2	1.22

element is constant on the 3 individual regions of the mesh. For the ratios given above, the size of an element on the wall is twice the size of an element on the hemisphere. The number of elements can be increased in a well defined manner with the above strategy, but the spacing of the elements is not optimal. Normally, elements of variable size are used to achieve higher accuracy with fewer elements. When the wall Green's function was used, a constant element size was chosen on the hemisphere.

The numerical calculations from the free-space Green's function are compared to Price's calculations [31] for a hemispherical protrusion in Table A.1. Price normalized the total force and the total torque by $\kappa\mu\pi R^2$ and $\kappa\mu\pi R^3$, respectively. The total dimensionless force and torque converge to the literature values faster than the locations for the points of zero shear stress converge to the literature values. The total force and torque converge to within 2.5% of the literature values with as few as 12 nodes. The literature values are matched with 60 nodes for the force and with 36 nodes for the torque. In contrast, the

Table A.2: The convergence of the dimensionless force, the dimensionless torque, and the location of the point of zero shear stress to the literature values from Price [31] for a hemispherical protrusion. Our numerical calculations in this table were done with the wall Green's function.

Wall Green's function - hemispherical protrusion			
N_{hemi}	Total dimensionless force on hemisphere $\frac{F_y}{\kappa\mu\pi R^2}$	Total dimensionless torque on hemisphere $\frac{T_z}{\kappa\mu\pi R^3}$	Angle on hemisphere where $\tau_w = 0$ (degrees)
4	4.38	2.42	76.9
6	4.33	2.43	78.0
8	4.32	2.44	73.0
10	4.31	2.44	74.2
12	4.31	2.44	74.1
16	4.31	2.44	73.7
20	4.31	2.44	73.4
26	4.30	2.44	73.4
32	4.30	2.44	73.3
64	4.30	2.44	73.2
Price [31]	4.30	2.44	73.2

literature values are not matched for the locations of the points of zero shear stress even with 96 nodes, but the values are within 1%. However, the literature values for the points of zero shear stress can be matched with 96 nodes if variable nodal spacing is used.

The numerical calculations from the wall Green's function are compared to Price's calculations for a hemispherical protrusion in Table A.2. The total dimensionless force and torque are within 2.5% of the literature values with as few as 4 nodes. The literature values are matched with 26 nodes for the force and with 8 nodes for the torque. The total number of nodes required for convergence is much less than for the free-space Green's function, but if one considers only the number of nodes on the hemisphere, then the convergence rate is about the same. Only one of the two locations for points of zero shear stress can be directly determined when the wall Green's function is used. As for the free-space Green's function, the convergence rate for the location of the zero-shear-stress point is slower than

Table A.3: Our calculation compared to literature values for the dimensionless force for a sphere touching or at various heights above a plane wall. The calculations were done using the wall Green's function with an increasing number of elements.

Wall Green's function - sphere above/touching wall					
N_{hemi}	Dimensionless force, $\frac{F_y}{6\kappa\mu\pi RH}$				
	H/R				
	1.0	1.1276	1.5431	2.3524	3.7622
4	1.7029	1.6202	1.441	1.279	1.167
6	1.6983	1.6170	1.440	1.278	1.167
8	1.6994	1.6163	1.439	1.278	—
10	1.7000	1.6161	1.439	—	—
12	1.7003	1.6160	—	—	—
16	1.7005	1.6160	—	—	—
20	1.7006	1.6160	—	—	—
26	1.7005	1.6159	—	—	—
32	1.7004	1.6159	—	—	—
64	1.7006	1.6159	—	—	—
100	1.7006	1.6159	—	—	—
128	1.7006	1.6159	—	—	—
O'Neill [30]	1.7009				
Goldman, Cox Brenner [33]		1.6160	1.4391	1.2780	1.1671

the convergence rate for the force or the torque. Unlike the free-space Green's function, however, the literature value for the zero-shear-stress point is matched by using 64 nodes.

For a sphere above a wall or touching a wall, only the wall Green's function was used to test the numerical accuracy of our code. A constant element size was chosen for the mesh. In Table A.3, the total dimensionless force for a sphere touching a wall is compared to the calculations of O'Neill [30], and the total dimensionless force for a sphere above a wall is compared to the calculations of Goldman, Cox, and Brenner [33]. Similar comparisons for the torque are presented in Table A.4. O'Neill and Goldman, Cox, and Brenner normalized the total force and the total torque by $6\kappa\mu\pi RH$ and $4\kappa\mu\pi R^3$, respectively, where H is the distance from the center of the sphere to the wall. With the force and torque normalized in this fashion, the dimensionless quantities approach 1 when the sphere is infinitely far from the wall.

Table A.4: Comparison of literature values for the dimensionless torque to the same quantities calculated by our boundary-integral program for the wall Green's function with varying numbers of elements.

Wall Green's function - sphere above/touching wall					
N_{hemi}	Dimensionless torque, $\frac{T_z}{4\kappa\mu\pi R^3}$				
	H/R				
	1.0	1.1276	1.5431	2.3524	3.7622
4	0.928198	0.94430	0.9652	0.9813	0.9882
6	0.936009	0.95038	0.9715	0.9874	0.9943
8	0.940387	0.95217	0.9731	0.9890	0.9959
10	0.942228	0.95291	0.9736	0.9895	0.9965
12	0.943058	0.95325	0.9739	0.9898	0.9968
16	0.943716	0.95352	0.9741	0.9900	0.9970
20	0.943900	0.95362	0.9742	0.9901	0.9970
26	0.943800	0.95368	0.9742	0.9901	0.9971
32	0.943731	0.95370	—	—	0.9971
64	0.943935	0.95372	—	—	—
100	0.943948	0.95372	—	—	—
128	0.943961	0.95372	—	—	—
O'Neill [30]	0.943993				
Goldman, Cox, Brenner [33]		0.95374	0.97419	0.99010	0.99711

In the first two columns in Tables A.3 and A.4, 128 nodes were used to try to match all of the significant digits of the literature values. For both the force and the torque, only 4 significant digits could be matched. However, the boundary-integral code produced stable results (*i.e.*, the results did not fluctuate wildly) up to 128 nodes. In the last three columns in Tables A.3 and A.4, we only tried to match 4 significant digits of the literature values. For the force, four significant digits could be obtained with 16 nodes or less, where fewer nodes were required when the sphere was farther from the wall. For the torque, four significant digits could be obtained with 128 nodes for a sphere touching a wall and with at most 26 nodes for all other cases. Except for the sphere touching the wall, moving the sphere farther from the wall did not improve the rate of convergence significantly.

Appendix B

Microelectrode Fabrication Procedure

The fabrication procedure for the microelectrode is summarized in Table B.1. The Berkeley Microlab equipment, the lithography masks, and the photosensitive polyimide and resists that were used in this study are summarized in Tables B.2, B.3, and B.4, respectively. Detailed information on general fabrication procedures and the equipment listed in Table B.2 is available in the U.C. Berkeley Microfabrication Manual, accessible via the World Wide Web (<http://argon.eecs.berkeley.edu:8080>).

B.1 Process issues

Corrosion-resistant materials should be used whenever possible in the electrochemical device because the electrolyte (0.5 M H_2SO_4 , 0.05 M FeSO_4 , 0.025 M $\text{Fe}_2(\text{SO}_4)_3$ —pH $\approx$ 0) used for the limiting-current experiments is corrosive. For this reason, titanium is used as an adhesion layer for the platinum electrode instead of chromium, which corrodes in the electrolyte. At pH=0, titanium forms a protective oxide at potentials greater than -0.4 V *vs.* the normal hydrogen electrode (NHE) [72]. Since the equilibrium potential of the redox couple for the limiting-current experiments is 0.64 V, up to 0.64+0.40=1.04 V of cathodic

Table B.1: Microelectrode fabrication process summary. For a description of equipment (such as the CPA) see Table B.2.

Step #	Step Description
1	Thermally grow 0.5 μm silicon dioxide by wet oxidation in furnace (Tylan1 or Tylan2).
2	Sputter 0.5 μm aluminum in CPA. Pattern using Mask 1 and Mask 2. Wet etch aluminum in 50 °C phosphoric acid in Sink8.
3	Deposit low-temperature oxide (LTO) on aluminum lines using the recipe lowtemp.psg in Tylan20. Pattern using Mask 3 and Mask 4. Plasma etch vias through oxide in Lam2.
4	Spin and pattern resist using Mask 5. Sputter 0.2 μm titanium in CPA. Sputter 0.2 μm platinum in Randex. Liftoff Ti/Pt layer by soaking in acetone.
5	Spin and pattern resist using Mask 6. Etch Ti/Pt layer in Ionmill to create microelectrodes.
6	Spin and pattern negative acting photosensitive polyimide using Mask 7A or Mask 7B to create a single polyimide protrusion or a polyimide protrusion array.
7	Spin and pattern resist using Mask 3 and Mask 4. Hard bake photoresist and do not strip. The resist serves as an extra corrosion-protection layer for the aluminum lines.
8	Dice wafer in Disco saw.

Table B.2: Equipment summary. For more information on the equipment listed in this table, refer to the U.C. Berkeley Microfabrication Manual, accessible via the world wide web (<http://argon.eecs.berkeley.edu:8080>).

Equipment name	Description
As200	A profilometer for measuring step heights.
CPA	A sputtering tool for depositing tungsten, titanium, or aluminum.
Curve Tracer	An analytical tool for measuring the current response to an applied alternating voltage.
Disco	A saw for cutting silicon or quartz wafers.
GCAWS1 and GCAWS2	10 to 1 projection printers for transferring a pattern from a mask to a wafer covered with photoresist. The mask does not contact the resist. More accurate alignment is possible than with the Quintel.
Ionmill	An ion-beam milling system for anisotropic etching of materials, including titanium and platinum.
IV	A probe station used to measure electrical resistivities.
Lam2	A plasma-etching tool for anisotropic etching of silicon dioxide.
Nanospec	An optical tool for measuring film thicknesses.
Quintel	A 1 to 1 contact printer for transferring a pattern from a mask to a wafer covered with photoresist. The mask contacts the photoresist.
Randex	A sputtering tool for depositing various dielectrics or metals, including titanium and platinum.
Sink4	A sink used during photolithography steps.
Sink8	A sink for wet etching aluminum, wet etching silicon dioxide, or cleaning.
Sink7	A sink for wet etching silicon nitride (<i>e.g.</i> , Si_3N_4) or cleaning.
Spinner1	A manual photoresist spinner.
Svgcoat	An automatic photoresist spinner for 100 mm wafers.
Tylan1 and Tylan2	Atmospheric-pressure furnaces for wet or dry thermal oxidation of silicon wafers.
Tylan20	Furnace for low-pressure chemical vapor deposition (LPCVD) of low-temperature silicon dioxide (LTO).
Vickers	An optical microscope used to measure line widths.

Table B.3: A summary of the masks used for the lithography steps.

Mask name	Description
Mask 1	Mask for creating alignment marks for rough positioning of the aluminum metalization layer (Figure B.1).
Mask 2	Mask for creating the aluminum metalization layer (Figure B.2).
Mask 3	First mask for creating vias through the silicon dioxide layer to the aluminum layer (Figure B.6).
Mask 4	Second mask for creating vias through the silicon dioxide layer to the aluminum layer. Also for clearing openings through the final protective photoresist layer to the aluminum layer (Figure B.7).
Mask 5	Mask for creating the 0.5 cm by 0.5 cm square platinum buffer electrode. Also for clearing openings through the final protective photoresist layer to the platinum electrode (Figure B.9).
Mask 6	Mask for creating the microelectrodes (Figure B.10).
Mask 7A	Mask for creating the polyimide protrusion array (Figure B.11).
Mask 7B	Mask for creating a single polyimide protrusion (Figure B.12).

Table B.4: A summary of the photoresists and the photosensitive polyimide that were used.

Name	Description
7020 polyimide	A negative-acting photosensitive polyimide from OCG Microelectronic Materials, Inc. QZ3501 developer, QZ3512 rinse from OCG is also required.
OCG 825 photoresist	Positive photoresist from OCG Microelectronic Materials, Inc.
s1400-31 photoresist	Positive photoresist from Shipley (now called s1818 photoresist).

polarization can be applied during the experiments without corroding the titanium, which gives a sufficiently large potential window for the electrochemical study (see Section 3.3). The chromium in previous microelectrodes (used by Dees [44] and Whitney [45]) tended to corrode. Sutija [5] improved the process by switching to titanium.¹ Titanium/platinum is probably the ideal combination for the working-electrode material. However, it is fortunate that the platinum step occurs relatively late in the process because platinum is difficult to pattern.

Although aluminum ($2.65 \mu\text{ohm-cm}^2$) corrodes in the electrolyte and although aluminum cannot be protected from the electrolyte by impervious thin films of silicon dioxide or silicon nitride (see next paragraph), it is used instead of platinum as the initial metalization layer because aluminum is easy to pattern. It is important to have an easy process because only 1 device is produced per wafer. Other possible materials for the initial layer either complicate the process (Pt, Au, TaSi_x , W) or are not conductive enough (phosphorus- or boron-doped Si; $\sim 100 \mu\text{ohm-cm}$ for 10^{21} atoms of P or B per cm^3 [74, page 31]). Aside from being difficult to pattern, platinum ($10.6 \mu\text{ohm-cm}$) can only be deposited on 1, 100 mm wafer at a time by sputtering in the Randex (see Table B.2) in the Berkeley Microlab. Gold ($2.35 \mu\text{ohm-cm}$ bulk) is easier to pattern than platinum and it is impervious to our electrolyte like platinum, but it also can only be deposited on 1, 100 mm wafer at a time by evaporation in the Berkeley Microlab. As an additional complication, platinum and gold require adhesion layers of titanium both above and below these layers. Whitney [45] tried TaSi_x ($15.5 \mu\text{ohm-cm}$) in place of aluminum because TaSi_x forms a protective oxide [72] in the electrolyte, but her devices did not work for reasons that were not identified. Like Pt and Au, however, TaSi_x can only be deposited on 1 wafer at a time in the Randex in the Berkeley Microlab. Because of its high melting point, tungsten can be protected from the electrolyte by an impermeable Si_3N_4 film deposited by chemical vapor deposition, tungsten can be sputtered on several wafers simultaneously in the CPA, and tungsten is used in

¹Whitney used titanium in a few microelectrodes, but these devices did not work [45].

²Unless otherwise mentioned, all resistivities are from [73] and are for bulk materials, not thin films.

standard processes in the Berkeley Microlab. Unfortunately, equipment problems prevented us from fabricating devices using tungsten. Even if all the equipment were operational, however, aluminum is still easier to use from a processing standpoint. Aluminum has excellent adhesion properties, it is easy to pattern, and several wafers can be sputtered simultaneously in the CPA.

Aluminum cannot be protected from the electrolyte by impervious silicon dioxide or silicon nitride thin films because aluminum melts at 660 °C [73]. Silicon nitride (Si_3N_4) is deposited by chemical vapor deposition at 800 °C and low temperature oxide (or LTO, which is silicon dioxide deposited by chemical vapor deposition) is annealed at 1000 °C. Of the above two films, the silicon nitride offers superior resistance to electrolyte penetration. When aluminum is the initial metalization layer, SiN_xH_y can be deposited by plasma enhanced chemical vapor deposition (PECVD) at 300 °C or LTO can be deposited at 400 °C (without an annealing step). These films offer some protection for the aluminum lines, but they are not sufficient to protect the aluminum without the hard-baked photoresist layer that is applied in the last processing step. The hard-baked photoresist does not protect the aluminum lines in the areas where the platinum electrode is ion milled, and it would be beneficial to have an impervious silicon nitride or silicon dioxide film in these areas. The SiN_xH_y film probably offers a more protection than the unannealed LTO, but the LTO is significantly easier to deposit in the Berkeley Microlab. Sutija [5] developed and used the SiN_xH_y /photoresist combination. We developed and used the LTO/photoresist combination. Earlier microelectrodes used by Dees [44] had an LTO layer but no photoresist. When the devices failed (device lifetime is discussed in Appendix D), corrosion of the aluminum was sometimes visually apparent near the ion-milled openings. At other times, the failure mechanism was not apparent by visual inspection under an optical microscope and remains unknown.

B.2 The mask set and lithography

Schematics of the masks that were used for fabricating the device are shown in Figures B.1 to B.12. We designed the masks using a computer program called Xkic, and the computer-generated patterns were transferred to chrome masks with the help of the Berkeley Microlab staff. Grey or black areas on the mask schematics are areas where the chrome is etched away. The remaining chrome pattern is in white. Positive photoresists were used for all lithography steps with the exception of the step with the negative photosensitive polyimide. For positive resists, the resist is removed in the areas that are exposed to UV light. Hence, the chrome pattern on the mask is the same as the photoresist pattern that remains after development.

The dimensions that appear on the mask schematics refer to the feature sizes that would be produced on the device for perfect pattern transfer. When Mask 2 is used for contact printing (using the Quintel), the features sizes on the mask are the same as on the device. All other masks are used for 10 to 1 projection printing (using GCAWS1 or GCAWS2 in the Microlab), where the features on the masks are 10 times the size of the features on the device.

Projection printing should be used over contact printing whenever possible because alignment between layers is easier and more accurate (at least in the Microlab) and because problems with photoresist sticking to the mask are avoided. For example, a skilled user may be able to align features with 2 or 3 μm accuracy using the Quintel, but a novice would be able to align features with 1 μm accuracy using the GCAWS1 or GCAWS2. The main concern with alignment accuracy is in the second-to-last lithography step for which a 50 μm thick polyimide film is patterned. Since this lithography step requires the most work, it would be unfortunate to redo this step as a result of alignment problems. Projection printing could not be used for the aluminum metalization layer (Figure B.2) because a 5 cm $\times$ 5 cm die size is required, and the maximum die size that can be exposed in the GCAWS1 or GCAWS2 is about 1 cm $\times$ 1 cm.

Unless otherwise noted, OCG 825 photoresist was used. It was applied at 6000 rotations per minute (RPM) in an automatic photoresist spinner (the Svgcoat). Before each photoresist lithography step, the wafers were dried for 30 minutes at 120 °C and exposed to a hexamethydisilazane (HMDS) gas stream to improve adhesion of the resist to the substrate. Before the polyimide lithography step, the wafers were dried for 30 minutes at 120 °C, but they were not exposed to HMDS because HMDS has a severely adverse affect on polyimide adhesion. After developing photoresist, photoresist residue (which is generally not visible under a microscope) was removed from the patterned areas in a 50 W oxygen plasma for 1 minute (using the Technics-C), a process called descumming. Photoresist scum can cause unusually long wet etch times or poor electrical contact between metal layers. After descumming, the photoresist was hard baked (with the exception of the titanium/platinum "lift-off" step—Section B.6) for 1 hour at 120 °C.

B.3 Substrate preparation

A 0.5 μm thick silicon dioxide film is grown on 24, prime silicon wafers (100 mm diameter with 100 crystal orientation) by wet, thermal oxidation at 1000 °C (Tylan1 or Tylan2) to form an electrically insulating substrate for the subsequent processing steps. 24 is the maximum number of wafers that can fit in the furnace. It takes about 2.5 hours total for temperature ramp up, wet oxidation, N₂ anneal, and temperature ramp down. After the thermal oxidation is complete, the oxide thickness is measured with the Nanospec, an analytical tool used for determining film thicknesses from light-wave interference patterns. For the LTO etch step (see Section B.5), the progress of the etch is monitored by measuring the total oxide thickness (thermal oxide + LTO) in the Nanospec at the locations of process monitor 1 (PM1) labeled in Figures B.2 and B.3. The etch step is complete when the measured oxide thickness is less than the thermal oxide thickness.

B.4 The aluminum metalization layer

0.5 μm of aluminum is sputtered in the CPA (the aluminum target contains 2% silicon). About 5 wafers are processed at a time. The majority of the processing time is for pump down (~ 1 hour). The deposition rate is calibrated weekly by Microlab staff and is approximately $86,000 \text{ \AA}$ of $\text{Al} \times \frac{\text{cm}}{\text{min}}$ track speed.

To facilitate the use of the GCAWS2 in subsequent lithography steps, the aluminum is patterned in two steps. In the first step, photoresist is spun and exposed at two positions located 4.57 cm apart using the GCAWS2 and Mask 1. The patterned aluminum is wet etched in phosphoric acid at 50 °C (Sink8), and the wafers are rinsed and dried. In the second step, photoresist is re-applied and exposed using the Quintel and Mask 2. The patterned aluminum is wet etched again in phosphoric acid at 50 °C, and the resulting aluminum lines are examined for shorts by visual inspection under a microscope.

In the procedure described above, Mask 2 is roughly aligned (20 μm accuracy was sufficient) to the pattern from Mask 1 using the alignment mark in Figure B.5 (which shows a close up of the alignment marks on Mask 2) that is identical to the alignment mark in Figure B.1 (Mask 1). The other two alignment marks in Figure B.5 are for use with the GCAWS2 in subsequent lithography steps. These two alignment marks are easily found using the GCAWS2 in subsequent lithography steps because their position on the wafer was roughly defined when the alignment mark in Mask 1 was etched into the aluminum. If the step with Mask 1 were skipped, GCAWS2 could still be used in subsequent lithography steps, but the alignment marks placed with Mask 2 would be difficult to find. In other words, alignment marks that are initially placed using the GCAWS2 are easily found using the GCAWS2, but alignment marks that are initially placed using the Quintel are difficult to find using the GCAWS2.

The locations of the alignment marks in Figure B.5 are shown in Figure B.2, which shows Mask 2 in its entirety. In the figure, the alignment marks are designated by the label LAM, which stands for lithographic alignment mark, and the LAM are spaced 4.57 cm

apart. Also shown in Figure B.2 are the 22 aluminum lines for the microelectrodes (labeled 1 to 22) and the aluminum lines for the buffer electrode (labeled A to D). Lines 1 to 22 and A to D terminate at 26 aluminum pads near the edge of the device, where the external connections are made to 2 printed circuit boards (*cf.*, Figure 3.10). The other ends of the aluminum lines terminate at 26, 30 $\mu\text{m} \times 30 \mu\text{m}$ aluminum pads near the center of the device. The central termination points of lines A to D are shown in the magnified view in Figure B.3, and the central termination points of lines 1 to 22 are shown at greater magnification in Figure B.4. The width of lines 1 to 22 decrease from 100 μm (Figure B.2) to 30 μm (Figure B.3) to 10 μm (Figure B.4) from the pads near the edge of the wafer to the pads near the center of the device.

The central plus symbol (+) in Figure B.4 is the location for a polyimide protrusion, and the aluminum pads are arranged in a cross pattern around this symbol. The pads are grouped in sets of 6 and 5. In each set of 6, the closest microelectrode to the central plus symbol is 100 μm (center-to-center), and, in each set of 5, the closest microelectrode to the central plus symbol is 125 μm (center-to-center). The center-to-center distance between adjacent aluminum pads within each set is 50 μm . This arrangement of the pads allows the density of data points to be doubled by reversing the flow direction during an experiment.

Several other features besides the aluminum lines are created by Mask 2. The extra features that were used in the final process are labeled in Figures B.2 and B.3. First, flow-cell alignment marks (FCAM) are labeled in Figure B.2. These are 4 aluminum squares located 1.347 cm apart in the direction transverse to the direction of the flowing electrolyte in the electrochemical experiments. To align the flow cell to the microelectrode device, the outer edges of the flow cell are aligned to the inner edges of the FCAM. A second feature, labeled in Figure B.2, is an arrow which was used for determining wafer orientation. Finally, process monitor number 1 (PM1) is labeled. As described in Section B.3, the oxide thickness (thermal oxide + LTO) is measured at PM1 to determine when the LTO etch is finished. In Figure B.3, the measurement locations for PM1 are outlined by 4 square rings of aluminum. In Figure B.2, the measurement locations for PM1 are adjacent to the

aluminum pads labeled A, D, 4, and 11 near the edge of the device.

B.5 Low-temperature-oxide (LTO) deposition and patterning

After patterning the aluminum lines, LTO is deposited on the aluminum lines in Tylan20 (recipe name: lowtemp.psg). Five wafers are usually taken through this step. This is a nonstandard process that we developed in the Microlab. The only difference from the usual recipe (vdoltoc) is that the deposition temperature was reduced from 450 °C to 400°C because this is a safer temperature to deposit LTO on aluminum (bulk aluminum melts at 660 °C). Before placing the wafers in Tylan20, the wafers are cleaned by soaking in acetone (10 minutes) and then rinsed clean (Sink7). One micron of LTO is deposited ($\sim 0.8 \mu\text{m}/\text{hour}$). The total oxide thickness (thermal oxide + LTO) is then measured using the Nanospec at the PM1 locations (see Figures B.2 and B.3). Since the thermal oxide thickness was previously measured at the PM1 locations, the LTO thickness can be determined by difference. Two of the PM1 locations near the center of the wafer (the top right and the bottom left in Figure B.3) are near to process-monitor number 2 (PM2), which is used to determine when the Ti/Pt etch step is finished (see Section B.7). PM2 first appears in Figure B.10 (Mask 6). PM1 and PM2 do not need to be in the exact same position because the oxide thickness varies slowly with position on the wafer.

Next, photoresist is spun on the wafer and exposed in GCAWS2 using Masks 3 and 4 (Figures B.6 and B.7). Mask 3 is used to create vias through the oxide for electrical connection to the microelectrodes and to the buffer electrode. Mask 3 also creates a square opening in the photoresist for the PM1s in Figure B.3. Mask 4 is used to create vias through the oxide for the outer aluminum pads and for the PM1s in Figure B.6 using six exposures, the positions of which are shown schematically in Figure B.8. The LTO is not etched from the entire aluminum pad so that the 100 μm lines are not exposed. This protects the 100 μm lines from accidental exposure to electrolyte. The aluminum pads are sufficiently large

so that they can withstand temporary accidental exposure to the electrolyte. The LTO is plasma etched in Lam2 ($\sim 0.7 \mu\text{m}/\text{minute}$), and the oxide thickness is measured at the PM1s using the Nanospec. Plasma etching is continued until the oxide thickness is less than the thermal oxide thickness. Finally, the photoresist is stripped, and the wafers are rinsed clean.

B.6 The titanium/platinum “lift-off” step

In this step, the titanium and platinum layers are sputtered and patterned using a lift-off procedure. In the lift-off procedure, the the Ti/Pt layer is sputtered on top of a patterned photoresist layer. The photoresist is then dissolved in acetone, and the Ti/Pt layer that was above the photoresist peels or “lifts” off. Five wafers can be taken through this step in about 2 to 3 days. The end result is a $0.5 \text{ cm} \times 0.5 \text{ cm}$ square thin-film layer of titanium ($0.2 \mu\text{m}$) and platinum ($0.2 \mu\text{m}$) which short circuits all of the aluminum lines together. The individual microelectrodes are not electrically isolated until after the ion-milling step. Note that $0.2 \mu\text{m}$ of titanium is a very thick adhesion layer (about 5 nm is sufficient for adhesion), but the additional thickness provides protection for the aluminum lines. Metal films which are too thin are porous to electrolyte.

The lift-off procedure was adapted from the procedure described in detail at the end of the equipment manual for the Randex. Briefly, 2 layers of photoresist are spun (6000 RPM, s1400-31 resist) with a soft bake after each spin. The wafers are then soaked in chlorobenzene for 10 minutes and exposed in GCAWS2 using Mask 5 (Figure B.9). It is important to descum the wafer with a 50 W oxygen plasma after developing the photoresist pattern so that the Ti/Pt layer will come into good electrical contact with the aluminum lines.

Next, $0.2 \mu\text{m}$ of titanium is sputtered in the CPA. The titanium is sputtered in two passes ($0.1 \mu\text{m}$ per pass) to prevent the wafer from overheating and burning the photoresist. Between passes, the wafers are cooled by venting the load-lock chamber. The wafers are

then removed from the CPA, exposing the titanium to air, and placed into the Randex to sputter the platinum. It is unorthodox to expose the titanium to air because an oxide layer forms. The titanium and platinum could both be sputtered in the Randex without exposing the wafer to air, but it is more difficult to deposit thick films in the Randex than the CPA because the photoresist heats up faster in the Randex. To prevent the photoresist from overheating in the Randex, 20 passes are used. Between passes, the wafers are allowed to cool for 1 minute with the plasma off, but the chamber is not vented. Because 20 passes are required and because only 1 wafer can be processed in the Randex, it is time consuming and tedious to take multiple wafers through this step.

After sputtering, the wafers are placed into acetone, and the Ti/Pt layer over the photoresist lifts off when the photoresist dissolves. Ultrasonic agitation speeds up the process. At this stage, the aluminum lines are electrically shorted, and the resistance of the individual lines can be tested without damaging the Ti/Pt layer using a probe station called the IV. To measure the resistivity of line 1 (see Figure B.2), for example, one probe is placed on pad 1 and the other probe is placed on pad C, and the resistance is measured using an ohmmeter. Since the resistance of line C and the contact resistance between the probes and the aluminum pads are much less than the resistance of line 1, the measured value is approximately equal to the resistance of line 1.

If the resistance of lines 1 to 22 is significantly greater than 100 ohms, the contact between the aluminum lines and the Ti/Pt layer is poor. The contact is easily improved by applying an alternating current with the Curve Tracer, which anneals the contact by resistive heating. The maximum potential is set to 15 V, and the maximum current is set to 20 mA. Every contact was treated in this manner. The Curve-Tracer procedure does not work as well for the connections between lines A or D and the Ti/Pt layer because the contact area is relatively large for these lines. As a result, the resistive heating is not as intense. Fortunately, the contact resistance could be reduced to acceptable values. A furnace anneal could have been used as a back-up procedure if the above procedure had

failed.³ The total resistance in parallel between the Ti/Pt layer and lines A, B, C, and D was typically 0.5 ohms.

B.7 Ion milling the titanium/platinum bilayer

In this step, the Ti/Pt layer was segmented into microelectrodes by ion milling, the highest-resolution technique for patterning this bilayer. Photoresist is spun and exposed in GCAWS2 using Mask 6 (Figure B.10). If the pattern were transferred perfectly to the Ti/Pt layer, the microelectrodes would be 49 μm square because the openings in the photoresist created by Mask 6 are ideally 1 μm wide. However, the openings are widened by about 0.5 μm during ion milling resulting in 48.5 μm square microelectrodes. Two round holes are also etched into the corner of the Ti/Pt layer (see Figure B.10). These holes constitute process monitor number 2 (PM2).

The machine used for this step is called the Ionmill. As with the Randex, only 1 wafer can be loaded into the Ionmill, and 5 wafers can be processed in about 2 to 3 days. Before loading a wafer, the bottom of the wafer is coated with a slurry of high-vacuum oil and aluminum powder to improve thermal contact to the platform on which the wafer sits. The etch takes about 18 minutes total (1.3×10^{-3} Pa argon pressure, 0.6 kV ion-acceleration potential), but the etch is stopped every 6 minutes for venting the Ionmill to prevent the photoresist from overheating.

After 18 minutes, the openings for the microelectrodes and PM2 are visually examined to determine whether the Ti/Pt layer has been cleared from these areas. If the etch appears to be complete, the oxide thickness at PM2 is measured using the Nanospec to check whether it is less than the oxide thickness at the corresponding PM1 after the LTO deposition step. If it is less, then a third check is performed. The photoresist on the outer aluminum pads is removed with a Q-tip soaked in acetone, and each aluminum line is checked for electrical isolation using the IV probe station. If any of these tests are

³The furnace temperature should be less than 400 °C. Temperatures higher than 400 °C would change the film properties of the LTO since the LTO was deposited at 400 °C.

not passed, the wafers are etched for another 1 or 2 minutes in the Ionmill with the aluminum pads covered by glass slides if necessary. The glass slides are held in place using the oil-aluminum powder slurry. If all tests are passed, the photoresist is stripped in acetone. Recalcitrant resist can be removed by lightly scrubbing with a Q-tip in the areas away from the microelectrodes. Recalcitrant resist on the microelectrodes is removed by a low-power (50 W) oxygen plasma. If a power greater than 50 W is used, the photoresist may become so recalcitrant that it cannot be removed without destroying the device.

B.8 Making the polyimide protrusions

A procedure was developed for fabricating 50 μm tall polyimide protrusions using 7020 negative-acting photosensitive polyimide (OCG Microelectronic Materials, Inc.). The procedure is given in detail since the 7020 polyimide is not covered in the U.C. Berkeley Microfabrication Manual.

B.8.1 Materials

1. Disposable plastic pipets, about 0.8 cm in diameter, with the tips cut off. The tips need to be cut off in order to pipet the viscous polyimide.
2. Two air brushes located near Sink4 in the Berkeley Microlab for applying the developer and rinse. The pressure of the air brushes should be adjusted to 1 atm gauge to prevent excess solvent from volatilizing during application.
3. The bottom half of a blue wafer-carrier box capable of holding 50, 100 mm wafers (or any other container of this approximate size that will not dissolve in the developer or rinse). The container should be as large as possible but must still fit into the sink in Sink4.
4. A platform to hold the wafer at approximately 45 ° in the blue box. We used a piece of aluminum with a step milled into it to create a lip for the wafer to rest on.

5. 7020 polyimide, QZ3501 developer, QZ3512 rinse from OCG.
6. A freezer to store 7020 polyimide at $< 0^{\circ}\text{C}$. The polyimide cross links relatively fast at room temperature.
7. An oven with an automatic temperature controller and a nitrogen feed. Such an oven is available in the "old lab" in the Berkeley Microlab.

B.8.2 Pre-spin procedure

1. Remove 7020 polyimide from the freezer, and allow it to equilibrate to room temperature for at least 6 hours. The bottle of polyimide should not be opened while the bottle is cool because condensed moisture ruins the polyimide's properties.
2. Adjust the hot-plate temperatures to 80 and 100°C . Allow 1 hour for hot plates to equilibrate.
3. Dry substrate in 120°C oven for 30 minutes. Skipping this step will adversely affect adhesion. Do NOT use HMDS because the polyimide will not adhere to a substrate coated with HMDS.

B.8.3 Spin procedure

The manual spinner is used (Spinner1). The following procedure produces a $25\text{ }\mu\text{m}$ thick film on the first coat. Each additional coat adds about $30\text{ }\mu\text{m}$ of thickness. Generally, longer spin times produce more uniform but thinner films. Relative to photoresist, polyimide thickness is very sensitive to spin time.

1. The settings for 500 RPM and 1000 RPM for Spinner 1 are established using a dummy wafer. Set the spin time to 45 seconds using a stopwatch. Load a real wafer.
2. Fill a plastic pipet with approximately 3 to 4 ml of polyimide. Start wafer spinning at 500 RPM. Dispense the polyimide slowly in the center of the wafer for a period of

about 10 to 15 seconds. The polyimide should spread over about 3/4 of the 100 mm wafer diameter at the low spin speed. Stop the spinner. Quickly adjust the setting to 1000 RPM, and spin for an additional 45 seconds.

3. Soft bake on hotplate (vacuum chuck on) at 80 °C for 5 minutes and 100 °C for 5 minutes. Allow the polyimide to cool for 5 minutes. The polyimide should be tack free.
4. For the second layers, repeat step 2 and change the soft-bake times in step 3 to 80 °C for 5 minutes and 100 °C for 10 minutes. The uncured thickness after 2 coats should be about 55 μm . The thickness is reduced by about 10% after a partial cure.

B.8.4 Exposure procedure

The polyimide is exposed using the GCAWS2 projection printer with Mask 7A for a protrusion array (Figure B.11) and with Mask 7B for a single protrusion (Figure B.12). The circular openings in each mask are 90 μm in diameter. However, the diameters of the resulting polyimide protrusions are slightly larger than 90 μm at the base of the protrusions and slightly smaller than 90 μm at the top of the protrusions. The actual diameters at the base and at the top of some protrusions in actual devices are given in the captions in Figures 3.1 and 3.2. The larger diameters at the base could be from overexposure in the GCAWS2. The smaller diameters at the top could be from overdevelopment using the QZ3501 developer, but this seems unlikely since the final diameter is stable even after excessive overdevelopment (2 to 3 times the minimum development time). The polyimide array has a square pitch, 318 μm along the square edges and 450 μm along the square diagonals.

Since the 7020 polyimide is the most sensitive to g-line ultraviolet radiation, the GCAWS2 (a g-line stepper) was used as the exposure tool. However, since the polyimide is very sensitive, the GCAWS1 (an i-line stepper) could also be used without adjusting the exposure time. The exposure time that was used for 50 μm thick polyimide layers was 0.4

seconds.⁴

Automatic wafer handling failures may occur on GCAWS1 or GCAWS2 because of the thick polyimide lip that accumulates on the wafer edges. In hindsight, the lip could have been removed by placing Kapton tape on the wafer edges before the polyimide was spun and removing the tape after the final soft bake. The polyimide must be tack free before they are loaded into GCAWS1 or GCAWS2.

B.8.5 Development procedure

Development times assume a 55 μm thick soft-baked film thickness.

1. Place the bottom half of the blue wafer carrier box in the bottom of Sink4. The box is used to prevent developer or rinse from flowing down the drain. Put the wafer on the metal wafer holder and place the holder into the blue box at approximately a 45 ° angle. Placing the box in the bottom of the sink in addition to reducing the air brush gauge pressure to 1 atm prevents volatiles from escaping Sink4. The solvent used for the developer and rinse is butyl acetate, which is not nearly as toxic as xylene, which was used previously.
2. Spray develop the polyimide for 2 minutes followed by a 20 second overlap, where the rinse and developer are sprayed simultaneously. Finally, spray the rinse for 30 seconds by itself. Dry the wafer with nitrogen (water rinsing is not necessary). Overdeveloping should not be problematic.
3. Examine the pattern under a microscope to check whether the polyimide was completely removed during the development step. The polyimide thickness can also be checked using the microscope. At all magnifications, 1 dial unit on the focus-adjustment knob equals 1 micron. The thickness measurements are more accurate at

⁴On nonopaque substrates such as glass or quartz this time should be reduced to about 0.1 seconds to reduce reflections.

higher magnifications because the depth of focus is more narrow. Continue developing if necessary.

4. Dispose of waste developer and rinse in the trichloroethane (TCA) waste bottles.

B.8.6 Procedure for partially curing the polyimide

A partial cure under nitrogen is obtained at 120 to 150°C for 1 hour. Although a nitrogen atmosphere is not necessary at temperatures less than 150°C, the nitrogen is used in case of temperature overshooting. After a partial cure, the polyimide is not fully imidized, but the polyimide is resistant to our electrolyte, and the polyimide side walls remain vertical. Also, about 10% of the thickness is lost from the partial cure, reducing the 55 μm thick soft-baked polyimide to 50 μm .

B.9 Adding the protective photoresist layer

The final lithography step is to add a layer of photoresist to protect the aluminum lines from the corrosive electrolyte. Standard OCG 825 photoresist is applied at 6000 RPM using the Svccoat. The polyimide protrusions do not adversely affect this low-resolution lithography step. Openings through the photoresist for the outer aluminum pads and the platinum electrode are created using Mask 4 (Figure B.7) and Mask 5 (Figure B.9), respectively, by projection printing with the GCAWS2. Six exposures are required for Mask 4 as illustrated in Figure B.8. Finally, the photoresist is hard baked for two hours at 120 °C.

B.10 Dicing the wafer

The Disco saw is used to cut the wafer into a 5.258 cm by 7.493 cm rectangle that fits into the flow-cell apparatus. The Disco will cut completely through the wafer if the wafer is placed on dicing tape and if the blade is set to 0.1 mm above the saw table. The side wall of the cut is nearly vertical, which is ideal for sealing the device in the flow-cell

apparatus.

Figure B.1: Mask 1: for creating alignment marks for rough positioning of the aluminum metalization layer.

Figure B.2: Mask 2: for the aluminum metalization layer. Close ups of the central region of this mask are shown in Figures B.3 and B.4, and a close up of the lithography alignment marks (LAM) is shown Figure B.5. The Al lines for the buffer electrode are labeled A to D. The Al lines for the microelectrodes are labeled 1 to 22.

Figure B.3: First close up view of the central region of Mask 2. The lines labeled A to D correspond to the lines labeled A to D in Figure B.2. PM1 is visible in this view.

Figure B.4: Second close up view of the central region of Mask 2. The lines labeled 1 to 22 correspond to the lines labeled 1 to 22 in Figure B.2.

Figure B.5: Close up view of lithography alignment marks (LAM) for Mask 2.

Figure B.6: Mask 3: first mask for etching the LTO. This mask is used to make openings through the LTO to the aluminum lines that terminate near the center of the device. The etch step is monitored using process monitor 1 (PM1).

Figure B.7: Mask 4: second mask for etching the LTO. This mask is used to make openings through the LTO to the aluminum pads where the external connections are made near the edge of the device. Six automated exposures are required using this mask.

Figure B.8: The six locations where mask 4 is exposed in relation to the aluminum pattern. The oxide thickness is monitored at the locations marked PM1. The LTO is not entirely removed from the outer aluminum pads.

Figure B.9: Mask 5: the mask for the Ti/Pt liftoff step. This mask is used to create the 0.5 cm square Pt buffer electrode.

● PM2

Figure B.10: Mask 6: for segmenting the Ti/Pt layers into microelectrodes by ion milling.

Figure B.11: Mask 7A: for creating the polyimide array. The circles are 90 μm in diameter and are arranged in a square array. One side of the square is 318 μm , and the diagonal is 450 μm . Only 1 exposure is required to create the entire array.

Figure B.12: Mask 7B: for creating a single polyimide protrusion.

Appendix C

Theoretical Limiting-Current Curves for a Ferric/Ferrous Redox Couple

Below, simple equations are derived for computing theoretical limiting current curves for the reaction

The limiting current curves are the total electrode current plotted against the potential difference between the working electrode and the reference electrode, $\Delta\Phi_{\text{total}}$, which is given by

$$\begin{aligned} \Delta\Phi_{\text{total}} &= \Phi_{\text{working}} - \Phi_{\text{reference}} \\ &= \text{OCP} + \Delta\Phi_{\text{ohmic}} + \eta , \end{aligned} \quad (\text{C.2})$$

where OCP is the open circuit potential, $\Delta\Phi_{\text{ohmic}}$ is the ohmic drop, and η is the total overpotential. The total overpotential is further defined by

$$\eta = \eta_s + \eta_c , \quad (\text{C.3})$$

where η_s is the surface overpotential and η_c is the concentration overpotential. The ohmic drop is estimated by

$$\Delta\Phi_{\text{ohmic}} = \rho iW, \quad (\text{C.4})$$

where W is the channel width (the distance between the working electrode and counterelectrode) and ρ is the resistivity.

The current density (as taken from [52, problem 20.4]) for the ferric-ferrous redox reaction is given by

$$i = i_0^\infty \left(\frac{C_{b0}}{C_\infty} \exp \left[\frac{\alpha_a F}{RT} \eta \right] - \frac{C_{a0}}{C_\infty} \exp \left[-\frac{\alpha_c F}{RT} \eta \right] \right), \quad (\text{C.5})$$

where C_∞ represents the bulk concentrations of both Fe^{2+} and Fe^{3+} which are the same, i_0^∞ is the exchange current density for the bulk electrolyte concentrations, and α_a and α_c are the apparent anodic and cathodic transfer coefficients. C_{b0} and C_{a0} are the concentrations of Fe^{2+} and Fe^{3+} , respectively, at the surface of the electrode. To simplify the mathematics, it is assumed that $\alpha_a = \alpha_c = 0.5$, which is consistent with the transfer coefficients reported in the literature (~ 0.4 to 0.6) [49].

The surface concentrations can be written in terms of the bulk concentration using an average mass-transfer coefficient, k . If the same value for k is used for both species, the relations are

$$\begin{aligned} i &= nkF(C_\infty - C_{b0}) \\ &= nkF(C_{a0} - C_\infty), \end{aligned} \quad (\text{C.6})$$

where F is Faraday's constant, and n is the number of electrons transferred. Substituting $n = 1$ and equations C.6 into equation C.5 and noting that

$$\frac{i_0^\infty}{i_l} = \frac{i_0^\infty}{kFC_\infty} \quad (\text{C.7})$$

finally gives

$$i = i_0^\infty \frac{(\exp [\frac{0.5F}{RT} \eta] - \exp [-\frac{0.5F}{RT} \eta])}{\left[1 + \frac{i_0^\infty}{i_l} (\exp [\frac{0.5F}{RT} \eta] + \exp [-\frac{0.5F}{RT} \eta]) \right]}, \quad (\text{C.8})$$

where i_l is the limiting current. Equation C.8 defines the limiting-current curves, but it does not predict the potential at which hydrogen is evolved.

If i were plotted against η instead of $\Delta\Phi_{\text{total}}$ (*i.e.*, if ohmic drop were subtracted), the shape of the limiting-current curves would only depend on the ratio i_o^∞/i_l . Since both i_o^∞ and i_l are directly proportional to C_∞ , the ratio i_o^∞/i_l is independent of C_∞ . However, the ratio decreases with increasing Reynolds number because i_l increases and i_o^∞ stays the same. The ratio ranges from 1.52 at $\text{Re}=140$ to 0.18 at $\text{Re}=12600$. Equation C.8 is used to calculate the theoretical limiting current curves in Figure 3.14 in Chapter 3 both with and without ohmic drop. The parameters that were used are given in the figure caption.

Appendix D

The Current to the Entire Electrode with or without Protrusions

The current to the entire electrode can be estimated using an equation of the form

$$\langle \text{Sh} \rangle_{WL} = a \text{Re}^b \text{Sc}^{1/3} (W/L)^{1/3}, \quad (\text{D.1})$$

where the subscript " WL " indicates that the Sherwood number is averaged over the electrode width and length. Equation D.1 has the same form as equation 3.22, which applies in laminar flow, and equation 3.28, which applies in turbulent flow. These equations were derived for electrodes without protrusions, but we will also use them for electrodes with protrusions.

$\langle \text{Sh} \rangle_{WL}/(\text{Sc}W/L)^{1/3}$ is plotted against Re for the no-protrusion experiments in Figure D.1 (wafer 12), for the single-protrusion experiments in Figure D.2 (wafer 6), and for the protrusion-array experiments in Figure D.3 (wafer 8) over Reynolds numbers between 200 and 12000. The Schmidt number is higher for the no-protrusion experiments ($\text{Sc}=1950$) than for the single-protrusion or the protrusion-array experiments ($\text{Sc}=1615$) because the heat exchanger was not installed until after the latter two experiments were performed. For

Figure D.1: $\langle \text{Sh} \rangle_{WL} / (\text{Sc} W/L)^{1/3}$ vs. Re for the no-protrusion experiment (wafer 12). The Reynolds-number range is approximately 200 to 12000, and the Schmidt number is 1950. The circles represent data collected through 69.1 minutes, and the triangles represent data collected through 89.6 minutes. The solid lines are fits through the data, and the dashed lines are the expected behavior expressed by equations 3.22 and 3.28.

Figure D.2: $\langle \text{Sh} \rangle_{WL} / (\text{Sc} W/L)^{1/3}$ vs. Re for the single-protrusion experiment (wafer 6). The Reynolds-number range is approximately 200 to 12000, and the Schmidt number is 1615. The circles represent data collected through 21.2 minutes, and the triangles represent data collected through 53.5 minutes. The solid lines are fits through the data, and the dashed lines are the expected behavior expressed by equations 3.22 and 3.28.

Figure D.3: $\langle \text{Sh} \rangle_{\text{WL}} / (\text{Sc} W / L)^{1/3}$ vs. Re for the protrusion-array experiment (wafer 8). The Reynolds-number range is approximately 200 to 12000, and the Schmidt number is 1615. The circles represent data collected through 42.1 minutes, and the triangles represent data collected through 110.2 minutes. The solid lines are fits through the data, and the dashed lines are the expected behavior expressed by equations 3.22 and 3.28.

$Sc=1950$, the average temperature of the experiments was $\sim 25^{\circ}\text{C}$, and for $Sc=1615$ the average temperature was $\sim 30^{\circ}\text{C}$. The data obtained at relatively short times are marked with circular symbols (the first data set) while the data obtained at relatively long times are marked with triangles (the second data set). The times at which the last datum point was obtained for the first and second data sets are given in the figure captions, where the times are measured with reference to the beginning of data acquisition. The devices are exposed to the electrolyte for approximately 1 hour prior to data acquisition while the flow loop is degassed. For each set, the data were collected in the order of increasing Reynolds number.

The circular and triangular data symbols represent the total measured current, and the solid lines are fit through the circles. The dashed lines represent the expected total current based on the currents measured at the microelectrodes. Specifically, for the expected values, a laminar-flow diffusivity for ferric ions (*cf.*, Table 3.2) was calculated from the currents measured at the microelectrodes in the no-protrusion experiments (*cf.*, Section 3.4.4). Then, this diffusivity was used in equations 3.22 and 3.28 to generate the dashed lines. The diffusivity was corrected to 30°C using the Stokes-Einstein equation (equation 4.1) for the single-protrusion and the protrusion-array experiments. The values for a and b used for the solid and dashed lines are indicated in the figures.

For each experiment, the $\langle Sh \rangle_{WL}/(ScW/L)^{1/3}$ that were directly measured are greater than the expected values. For example, the data symbols are 30% to 50% above the expected values in Figure D.1. This difference is disconcerting because the total current and the microelectrode current are measured in the same experiment. The $\langle Sh \rangle_{WL}/(ScW/L)^{1/3}$ from the measured total current may be high because the current densities that were used to calculate the Sherwood numbers were based upon the electrode area within the inner flow-cell walls ($0.3175\text{ cm} \times 0.5\text{ cm}$). However, the entire electrode area ($0.5\text{ cm} \times 0.5\text{ cm}$) is actually exposed to electrolyte because the o-ring seals fall outside of the entire electrode area (see Figure 3.7). The full electrode area is 57% larger than the electrode area that falls within the inner flow-cell walls.

Table D.1: Best-fit calculations of the exponent b and the expected values for the exponent b corresponding to equations 3.22 and 3.28.

	"b" Laminar	"b" Turbulent
No Protrusion (wafer 12)	0.371	0.617
Single Protrusion (wafer 6)	0.352	0.516
Protrusion Array (wafer 8)	0.338	0.688
Expected	0.333	0.580

More attention should be given to the slope of the solid and dashed lines in Figures D.1 to D.3 than to the magnitude of the quantity $\langle Sh \rangle_{WL} / (ScW/L)^{1/3}$. In other words, the exponent b is more important than the coefficient a . The expected exponents and the exponents from the direct measurements (from the solid lines) are given in Table D.1. The greatest deviation from the expected laminar exponent is 11% for the no-protrusion case, and the greatest deviation from the expected turbulent exponent is 18% for the protrusion-array case. All of the exponents from the direct measurements are higher than the expected exponents, except for the turbulent-flow, single-protrusion exponent. From the analysis in Section 3.4.3, it was concluded that if b was to deviate from the expected value for turbulent flow, it should deviate on the high side. This suggests that the experimental error may be the greatest for the turbulent-flow, single protrusion experiments. However, the turbulent-flow, single-protrusion current distributions (Figure 3.19) were nearly the same, with the electrolyte flowing in either the S- or AS-directions, a more direct test which indicates that the current distributions were reasonably free of error.

Finally, the second data set (the triangular data symbols) always lies below the first data set (the circular data symbols), with the exception of the laminar-flow, protrusion-array

data (Figure D.3). Significantly lower values for the data in the second data set indicate that the device is beginning to fail because the electrode can no longer support a current. For example, for the single-protrusion experiments (Figure D.2), the device began to fail in the turbulent-flow regime when the second data set was being collected. Device failure probably results from corrosion of the aluminum metalization layer, but the mode of failure was not always discernible by visual inspection. For the laminar-flow, protrusion-array data, the second data set probably lies above the first data set because organic residue is removed from the electrode during the experiment. Once the residue is removed, the active electrode surface area increases and the total electrode current increases.

Appendix E

Nomenclature

Table E.1: Nomenclature

a	protrusion radius, cm
A	area, cm^3
C	a curve concentric with the protrusion
C_a	concentration of species a (ferric ions), mole/cm^3
C_{a0}	surface concentration of species a (ferric ions), mole/cm^3
C_{b0}	surface concentration of species b (ferrous ions), mole/cm^3
C_x, C_σ	constant unit vector coefficients
$\bar{C}_a$	bulk-phase concentration of species a , mole/cm^3
d_h	hydraulic diameter, cm
(D)	a curve
D	usage 1: a surface
D	usage 2: diameter of a circular pipe, cm
D_a	diffusivity of species a , cm^2/s
Det	determinant
Dis	discriminant
E	complete elliptic integral of the second kind
f	friction factor
f	force per unit area, $\text{g}/(\text{cm s}^2)$

F	usage 1: Faraday's constant, C/equiv
F	usage 2: complete elliptic integral of the first kind
F_j	total force on the protrusion, g cm/s ²
$\bar{F}_j$	total dimensionless force on the protrusion
F_j^p	total disturbance force on the wall or the protrusion, g cm/s ²
$\bar{F}_j^p$	total dimensionless disturbance force on the wall or the protrusion
$\mathfrak{F}_x$	function representative of the x component of $\mathbf{f}$, g/(cm s ²)
$\mathfrak{F}_\sigma$	function representative of the σ component of $\mathbf{f}$, g/(cm s ²)
$\mathfrak{F}_\phi$	function representative of the ϕ component of $\mathbf{f}$, g/(cm s ²)
$\mathbf{g}$	point force, g cm/s ²
G	free-space or wall Green's function, cm ⁻¹
h	protrusion height, cm
H	distance from the center of the sphere to the wall, cm
h_0	$h_0 = (x_0 - x_w)$, cm
i	current density, mA/cm ²
i_0	exchange current density, mA/cm ²
i_l	limiting current density, mA/cm ²
$\langle i \rangle_W$	current density averaged over the electrode width (W), mA/cm ²
$\langle i \rangle_{WL}$	current density averaged over the electrode width (W) and length (L), mA/cm ²
$\langle i \rangle_{y=-350 \mu\text{m}}$	average current density at microelectrode 1, assuming that the electrolyte is flowing in the S-direction, mA/cm ²
I	usage 1: current, mA
I	usage 2: instantaneous current, mA
I_{mn}	elliptic integrals (m and n run through x, σ, ϕ), cm ^{-m}
I_0	background current, mA
$\bar{I}$	time-averaged current, mA
I'	instantaneous deviation from the average current, mA
k	usage 1: constant
k	usage 2: mass transfer coefficient, cm/s
l	length along a curve, cm

L	usage 1: a curve parallel to the y axis
L	usage 2: length of electrode in flow direction, cm
L_h	hydraulic entry length, cm
L_e	mass-transfer entry length, cm
M	total number of elements under protrusion
$\mathbf{n}$	normal vector
n	number of electrons transferred
N	usage1: total number of elements on protrusion and wall
N	usage 2: nodal point
N	free-space or wall Green's function in cylindrical coordinates
OCP	open-circuit potential, V
p	pressure, Pa
Pe	Péclet number for the flow channel, $Pe = u_b d_h / D_a$
Pe_p	Péclet number based on the protrusion height and the shear rate at the wall, $Pe_p = \beta h^2 / D_a$
$\mathfrak{P}$	function representative of the pressure, Pa
Q	volumetric flow rate, cm^3/s
$Q_{\alpha\beta}, Q'_{\alpha\beta}$	kernel of the integral equations, cm^{-1}
r	$ \hat{\mathbf{x}} $, distance from the pole, cm
r_c	usage 1: distance from the point $(x_c, 0, 0)$, cm
r_c	usage 2: radius of curvature of a rounded corner, cm
r_{cyl}	radius at the top of the polyimide protrusions, cm
$\mathbf{R}$	residue, cm/s
R	usage 1: radius of curvature for spherical-type protrusions, cm
R	usage 2: $ \hat{\mathbf{X}} $, cm
R_λ	correlation coefficient; $\lambda=t, y$, or z (time, y direction, or z direction)
Re	Reynolds number for the flow channel, $Re = W u_b / \nu$
Re_p	Reynolds number based on the protrusion height and the shear rate at the wall, $Re_p = \beta h^2 / \nu$
Re'_p	Reynolds number based on the protrusion height and the velocity at the top of the protrusion, $Re'_p = V_{\text{top}} h / \nu$

s_a	stoichiometric coefficient for species a (negative for cathodic reactant)
dS	usage 1: differential area, cm^2
dS	usage 2: differential length along the curve S , cm
S	usage 1: distance along the trace of the protrusion and the wall, cm
S	usage 2: saddle point
Sc	Schmidt number
$\langle Sh \rangle_W$	Sherwood number averaged over the electrode width
$\langle Sh \rangle_{WL}$	Sherwood number averaged over the electrode width and length
t	time, s
$\mathbf{t}$	tangent vector
T	temperature, K
$\mathbf{T}$	stress tensor associated with the Green's function, cm^{-2}
T_z	total torque on a protrusion about the origin, $\text{g cm}^2/\text{s}^2$
Tr	trace
$\mathbf{u}$	velocity, cm/s
u_b	average flow-channel velocity, cm/s
u^*	friction velocity, cm/s
u_x	function representative of the x component of $\mathbf{u}$, cm/s
u_σ	function representative of the σ component of $\mathbf{u}$, cm/s
u_ϕ	function representative of the ϕ component of $\mathbf{u}$, cm/s
V	a unit volume, cm^3
V_{top}	velocity at top of protrusion, cm/s
W	width, height, and hydraulic diameter of flow channel, cm
x, y, z	coordinates ($x = X$, $y = Y - 0.25 \text{ cm}$, $z = Z - 0.15875 \text{ cm}$), cm
X, Y, Z	coordinates ($X = x$, $Y = y + 0.25 \text{ cm}$, $Z = z + 0.15875 \text{ cm}$), cm
x_w	x position of the wall, cm
$\mathbf{x}$	$\mathbf{x} = \mathbf{x}_i = (x_1, x_2, x_3) = (x, y, z)$, cm
$\hat{\mathbf{x}}$	$\hat{\mathbf{x}} = \mathbf{x} - \mathbf{x}_0$, cm
$\hat{X}$	$\hat{X} = (X = x - (2x_w - x_0), \hat{y}, \hat{z})$, cm
$\mathbf{x}_0$	usage 1: a point where the flow is not regular (pole), $\mathbf{x}_0 = (x_0, y_0, z_0)$, cm
$\mathbf{x}_0$	usage 2: a singular point, $\mathbf{x}_0 = (x_0, y_0, z_0)$, cm

Table E.2: Greek symbols

α	angle subtended from the top of a spherical-type protrusion to the wall
α_a	apparent anodic transfer coefficient
α_c	apparent cathodic transfer coefficient
β	shear rate, s^{-1}
Γ	gamma function
δ_{ij}	delta function
δ_m	mass transfer boundary layer thickness, cm
η	usage 1: dummy length variable, cm
η	usage 2: total overpotential, V
η_c	concentration overpotential, V
η_s	charge-transfer overpotential, V
κ	shear rate, s^{-1}
λ	time or position, s or cm
λ_0	reference time or position, s or cm
Λ_t	time scale of turbulence, s
Λ_y	length scale of turbulence in y direction, cm
Λ_z	length scale of turbulence in z direction, cm
μ	viscosity, $g/(cm\ s)$
ν	kinematic viscosity, cm^2/s
ξ	dummy length variable, cm
ρ	resistivity, ohm-cm
σ	radial direction for cylindrical coordinates, cm
σ_{ij}	stress tensor, $g/(cm\ s^2)$
τ_w	wall shear stress, $g/(cm\ s^2)$
τ_w^∞	undisturbed wall shear stress far from protrusion, $g/(cm\ s^2)$
$\Phi_{\text{reference}}$	potential of the reference electrode, V
Φ_{working}	potential of the working electrode, V
$\Delta\Phi_{\text{ohmic}}$	ohmic drop, V
$\Delta\Phi_{\text{total}}$	potential between working and counterelectrodes including ohmic drop, V
ψ	angle about the point $(x_c, 0, 0)$ from the x -axis

Table E.3: Subscripts

a	attachment
b	base of protrusion
c	center
i	infinity
i, j, k	indices representing Cartesian coordinates
l	limiting value close to boundary
p	protrusion
s	separation
w	wall
α, β	indices representing cylindrical coordinates

Table E.4: Superscripts

D	disturbance
F	free-space
IM	image
W	wall
∞	infinity
$+$	indicates quantity is dimensionless

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