PUNCH-SHEAR CHARACTERISTICS OF NANOCLAY AND GRAPHITE PLATELET 
REINFORCED VINYL ESTER PLATES, LAMINATED FACE SHEETS AND 
SANDWICH COMPOSITES UNDER LOW VELOCITY IMPACT

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ABSTRACT
This work describes the punch-shear response of nanoparticle reinforced vinyl ester plates, laminated face sheets and sandwich composites using Dynatup 8250 drop-weight impact test instrument according to the ASTM D3763 Standard. Tests were performed on 4” × 4” square plate specimens with fixed circular boundary condition, impacted by a hemispherical-head plunger with added mass. The impact load, displacement, energy plots and visual inspection of the post damaged specimens depicted the punch-shear characteristics of these composites.

Test results show more than 10% improvement in impact energy absorption with addition of 2.5 wt. pct. graphite platelets to pure vinyl ester. Maximum improvement in energy absorption (about 40%) was observed with Owens Corning HP ShieldStrand® glass fabric face sheets compared to the E-glass/vinyl ester. In another set of experiments with fly-ash based EcoCore® sandwiched in between E-glass/vinyl ester face sheets showed approximately 85% more energy absorption than with Tycor®, Balsa wood and PVC foam cores.

INTRODUCTION
Nanoparticle reinforced glass/carbon polymeric based composites and structural foams are being considered for use in military, new generation naval ships and critical infrastructure applications where lightweight damage tolerant structures are essential for blast, shock, impact mitigation. Prediction of damage, energy absorption and penetration resistance are important to develop stronger, safer and more cost-effective structures. Analyzing the rate sensitivity of these new material systems is essential for applications involving wide range of dynamic loading conditions. Gama et al. [1, 2] and Xiao et al. [3] performed quasi-static, ballistic and low velocity impact punch-shear tests to define the elastic and absorbed energies of composites as a function of penetration displacement. Shaker et al. [4] studied the failure mechanism of basket weave and 3-D braided Kevlar-fabric reinforced epoxy composites under low and high velocity impacts. Hosur et al. [5] carried out low velocity impact tests on quasi-isotropic CFRP composite laminates. This paper describes the punch-shear response of nanoparticle reinforced vinyl ester plates, laminated face sheets and sandwich composites using Dynatup 8250 drop-weight impact test system according to ASTM D3763 Standard [6]. Low velocity tests were performed on 4” × 4” square plate specimens with fixed circular boundary condition and impacted by a hemispherical-head plunger with added mass. The impact load, displacement, energy plots and visual inspection of the post damaged specimen described the failure characteristics and punch shear response of these composites.

MATERIAL DESCRIPTION
510A-40 brominated vinyl ester nanoparticle reinforced composite plates: Five different Derakane 510A-40 vinyl ester thermoset nanocomposites, reinforced with 1.25 and 2.5 wt. percent Cloisite 30B nanoclay and exfoliated graphite (xGnP) nanoplatelets, were manufactured at Michigan State University - Composite Materials and Structures Center.

Laminated woven fabric composite face sheets: Four different woven fiber fabric laminated composite face sheets were fabricated with Dow Derakane 510A-40 brominated vinyl ester resin by the VARTM process at the University of Alabama - Birmingham. The base specimen is a five-ply E-glass woven fabric with laminate schedule [(0/90)/(+45/-45)/(90/0)/(-45/+45)/(0/90)]. The second face sheet was prepared with same laminate configuration, but with 2.0 wt. pct. xGnP-15 exfoliated graphite platelets pre-mixed in the vinyl ester resin before fabrication. The third face sheet was made with five-layers of Owens Corning high performance HP ShieldStrand® glass fabric with similar laminate schedule and resin. The fourth face sheet was made with only three plies of FOE treated T-700 carbon fabric [(0/90)/(+45/-45)/(90/0)] laminate schedule in same matrix. Here the number of plies was reduced from five to three to keep stiffness of this carbon fabric laminate consistent with the other glass fabric face sheets.

Sandwich composites made with five-ply E-glass face sheets and light-weight cores: Six different kind of sandwich composites fabricated with 2” thick Tycor® (an
engineered 3-D fiber reinforced damage tolerant core from WebCore Technologies), poly-vinyl chloride (PVC) foam, balsa-wood and three types of fire-resistant EcoCore® (fly-ash based core material mixed with chopped JM3 and OC2 glass-fibers) sandwiched in between the five-ply E-glass/vinyl ester face sheets were fabricated at University of Alabama – Birmingham. The impact test specimens were cut in size of 4"x 4" (101.6 mm x 101.6 mm) each using bench saw from individual fabricated panels.

LOW VELOCITY IMPACT TESTS

The experiments were performed using Dynatup 8250 drop weight impact test system [Figure 1], according to the ASTM D3763 Standard. Specimen clamp assembly consists of parallel rigid steel plates with a 3" (76.2 mm) diameter hole in the center of each. Sufficient clamping force was applied to prevent slippage of the specimen during impact. Plunger assembly consists of a ½" (12.70 mm) diameter steel rod of 2" (50.8 mm) length with a hemispherical end of the same diameter positioned perpendicular to, and centered on, the clamp hole. Dynatup Impulse™ data acquisition systems are equipped with load and velocity transducers to provide data collection, analysis and reporting. Using an instrumented tup, the data acquisition hardware captures instantaneous load signals and transfers to the impulse software for further data processing. The velocity at impact is measured just prior to impact using a photoelectric-diode and flag system.

EXPERIMENTAL PROCEDURE

Three samples from each type of nanoparticle reinforced vinyl ester plates, laminated face sheets and sandwich composites were tested under low velocity impact and the average data considered for this investigation. Impact drop weight and height were determined such that velocity slowdown is less than 20% during the impact event as well as the applied impact energy was at least three times the energy absorbed by the specimen at peak load [1]. This configuration provided about 38 J of impact energy and 3.6 m/s impact velocity for the nanoparticle reinforced vinyl ester plates and about 185 J impact energy and 4 m/s impact velocity for the laminated face sheets and sandwich composites. A steel plunger with hemispherical end (0.5" dia. x 2" long) was used for penetrating the specimens with the required impact energy and velocity.

VISUAL INSPECTION

510A-40 brominated vinyl ester nanoparticle reinforced composite plates: The visual inspection of the specimen illustrates that the radial growth of damage centering impact point is less for pure vinyl ester [Figure 2.(i)] than its nanocomposites. Nanoclay reinforced composites are damaged equally on both faces [Figures 2.(ii) and 2.(iii)], whereas graphite platelet reinforced composites showed more damage on the rear than impact side [Figures 2.(iv) and 2.(v)]. In some cases of graphite platelet reinforced nanocomposites, fracture propagates very less on impact side. Penetration of plunger through the specimen required some more load due to the shearing friction between plunger wall and the inner surface of the punch through hole, which resulted to additional energy absorption.

Laminated woven fabric composite face sheets: Visual inspection of these specimens confirms that the radial growth of delamination was less for E-glass/vinyl ester face sheet [Figure 3.(i.b)] than HP- glass/vinyl ester face sheet [Figure 3.(iii.b)] and occurred at reverse side for both sheets. Due to opacity of E-glass/xGnP-vinyl ester and T-700 Carbon/vinyl ester face sheets, the occurrence of delamination was not visible [Figures 3.(ii) and 3.(iv)]. In case of T-700 Carbon/vinyl ester face sheets, carbon fiber strands were peeled off partially from back side [Figure 3(iv.b)]. The shredded fibers due to plunger penetration were clogged in the puncture hole.

Sandwich composites made with five-ply E-glass face sheets and light-weight cores: The visual inspection of the specimen depicts that the radial growth of delamination is least in tough core, whereas more in case of softer cores. E-glass/Tycor sandwich [Figures 4.(i.a) to 4.(i.c)] shows three different modes of failure due to impact on web-intersection, web-line and direct foam zones respectively. It can be observed that the softest foam-zone showed maximum delamination whereas the web-intersection allowed least delamination. Fly-ash based EcoCore is the toughest and has highest density among all. It showed less delamination as well as less depth of penetration [Figures 4.(iv) to 4.(vi)]. PVC and Balsa cores showed average performance with respect to delamination and puncture [Figures 4.(ii) and 4.(iii)].
RESULTS AND DISCUSSION

The Dynatup impulse data acquisition software provided instantaneous impact point displacement and applied load data. The load versus deflection data were plotted up to failure point for each tested sample. Corresponding cumulative energy absorption data were generated using Trapezoidal numerical integration method (Equation 1). In case of laminated woven fabric composite face sheets, absorbed energy was normalized-to-thickness (NTT) to eliminate the effects of specimen thickness variations and plotted accordingly.
The equation for energy absorption is given by:

\[ E(1) = E(-1) + 0.5 \times [L(1) + L(-1)] \times [D(1) - D(-1)] \quad \ldots (1) \]

Where,
- \( E(1) \) = Energy absorbed up to the current displacement data point,
- \( E(-1) \) = Energy absorbed up to the immediate former displacement data point,
- \( L(1) \) = Required load for the current displacement data point,
- \( L(-1) \) = Required load for the immediate former displacement data point,
- \( D(1) \) = Current displacement data point, and
- \( D(-1) \) = Immediate former displacement data point

Figures 6, 11, 16 show the superimposed load response and Figures 7, 12, 17 show energy response with respect to tup deflection. Load versus deflection plot shows two distinct phases of failure propagation for complete puncture [2]. These two phases are damage initiation and puncture propagation.

**Damage initiation phase:** The first phase, named as damage initiation phase, is observed from the moment of impact to the point of peak load, where the damage initiates with almost uniform deflection with some initial fracture peaks [Figure 5].

Pure vinyl ester and nanoclay reinforced vinyl ester show stiff but linear load-deflection response at this stage. A little change of slope explains fracture initiations and plastic flow [Figure 6]. Graphite platelet reinforced vinyl ester has distinctive multi-peak load fluctuations at this phase. This response showed large fracture generation at the rear side of the specimen. Energy absorption is carried out mainly at this phase [Figure 8].

All laminated face sheets showed a smooth elastic deformation with cloisse stiffness [Figure 11]. E-glass/vinyl ester face sheet showed marginally higher stiffness than that of the other configurations. HP-glass/vinyl ester face sheet sustained maximum peak load among all. E-glass/vinyl ester and T-700 Carbon/vinyl ester face sheets took more or less same amount of load before puncture. E-glass/xGnP-vinyl ester composite took least load in this phase. However, this face sheet fairly deflected during the damage initiation phase and hence absorbed maximum energy up to peak load same as HP-glass/vinyl ester face sheet; whereas T-700 Carbon/vinyl ester absorbed least energy [Figure 13].

The sandwich composites show five clear peaks indicating failure of each fiber lamina of the impact side face sheets up to peak load [Figure 16]. PVC sandwich fails at minimum peak load. All other sandwiches took approximately same amount of load at this phase. Energy absorption remained less for all sandwiches [Figure 18].

**Puncture propagation phase:** At the point of peak load, puncture is initiated and accomplished by rapid load-reduction. This phase can be identified as puncture propagation phase [Figure 5].

Vinyl ester nanocomposite plates showed sharp and smooth load-reduction. Comparatively harder and brittle graphite platelet reinforced nanocomposites absorbed less energy in this phase. Puncture propagation phase absorbed less energy due to short duration and material fragmentation occurred severely with some hinging effects [Figures 6 and 9].

Some prominent hinging effects of attached fiber fragments with the surface of the plunger are observed in case of all laminated face sheets. Only E-glass/xGnP vinyl ester composite showed comparatively smooth puncture propagation [Figure 11]. HP-glass/vinyl ester composite face sheet provided lot of resistance after peak load and continued to cause delamination. Hence the load-deflection plot shows a distinctive wavy plateau region at peak load. HP-glass/vinyl ester face sheet absorbed 60% more energy than E-glass/vinyl ester face sheet during the puncture propagation phase. E-glass/xGnP-vinyl ester and T-700 Carbon/vinyl ester showed comparative less energy absorption [Figure 14].

In case of sandwich composites, load reduction is very less and slow. Plunger could not penetrate the 2.25" thick sandwich specimen deeper than 0.6" (15 mm). Lot of hinges [Figure 16] depicts uneven resistance due to ripped fiber and core materials which influenced significant energy absorption after peak load. EcoCore showed the best energy absorption in this phase [Figure 19].
Table 1. Energy absorption of composite samples

<table>
<thead>
<tr>
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<th>Energy absorption (J)</th>
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<tbody>
<tr>
<td></td>
<td>Damage Initiation</td>
<td>Puncture propagation</td>
<td>Total</td>
<td></td>
</tr>
<tr>
<td>510A-40 brominated vinyl ester nanoparticle reinforced composite plates</td>
<td></td>
<td></td>
<td></td>
<td></td>
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<tr>
<td>Pure vinyl ester</td>
<td>9.05</td>
<td>6.22</td>
<td>15.27</td>
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<tr>
<td>1.25 wt.pct. Nanoclay</td>
<td>6.63</td>
<td>7.09</td>
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<tr>
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<td>5.65</td>
<td>7.78</td>
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<tr>
<td>1.25 wt.pct. Graphite</td>
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<tr>
<td>2.5 wt.pct. Graphite</td>
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<td>3.26</td>
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<tr>
<td>Impact energy = 185 J</td>
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<tr>
<td>Impact velocity = 4 m/s</td>
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Laminated woven fabric composite face sheets

<table>
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<td>Damage Initiation</td>
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<tr>
<td>E-glass/xGnP-15</td>
<td>12.81</td>
<td>8.35</td>
<td>21.16</td>
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<tr>
<td>HP-glass</td>
<td>12.13</td>
<td>16.00</td>
<td>28.13</td>
<td></td>
</tr>
<tr>
<td>T-700 Carbon</td>
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<td>7.53</td>
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<tr>
<td>Impact energy = 185 J</td>
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<tr>
<td>Impact velocity = 4 m/s</td>
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Sandwich composites made with five-ply E-glass face sheets and light-weight cores

<table>
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<th>Energy absorption (J)</th>
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<tbody>
<tr>
<td></td>
<td>Damage Initiation</td>
<td>Puncture propagation</td>
<td>Total</td>
<td></td>
</tr>
<tr>
<td>E-glass/ Tycor</td>
<td>32.70</td>
<td>54.30</td>
<td>87.00</td>
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<tr>
<td>E-glass/ PVC</td>
<td>29.22</td>
<td>52.28</td>
<td>81.50</td>
<td></td>
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<tr>
<td>E-glass/ Balsa</td>
<td>24.61</td>
<td>63.87</td>
<td>88.48</td>
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<tr>
<td>E-glass/EcoCore 0 wt.pct.</td>
<td>47.80</td>
<td>113.00</td>
<td>160.80</td>
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<tr>
<td>E-glass/EcoCore 4.5 wt.pct. JM3</td>
<td>34.65</td>
<td>121.10</td>
<td>155.75</td>
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<tr>
<td>E-glass/EcoCore 4.5 wt.pct. OC2</td>
<td>23.89</td>
<td>130.40</td>
<td>154.29</td>
<td></td>
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Impact energy = 38 J
Impact velocity = 3.6 m/s

Total Energy absorption: The total energy absorption was calculated as the sum of the energy absorbed for damage initiation and puncture propagation phases up to complete failure of the specimen.

Table 1 and bar charts [Figures 8-10, 13-15 and 18-20] of energy absorption at damage initiation and puncture propagation phases as well as the total energy absorption are provided for comparative investigation of the punch shear response of all types of vinyl ester nanocomposites, laminated face sheets and sandwich composites under low velocity impact.

Figure 6. Load-deflection response of vinyl ester nanocomposites

Figure 7. Energy-deflection response of vinyl ester nanocomposites
Nanoparticle reinforced vinyl ester plates: The first set of experiments on nanoparticle reinforced vinyl ester plates showed more than 10% improvement in impact energy absorption with the addition of 2.5 wt. pct. graphite platelets to pure vinyl ester. However, the nanoclay and 1.25 wt. pct. graphite platelet reinforcements showed a detrimental effect [Figure 10].

Laminated woven fabric composite face sheet: The second set of experiments on laminated composite face sheets showed thickness dependent punch-shear response. In this case the absorbed energy was normalized-to-thickness (NTT) to eliminate the effects of specimen thickness variations. Addition of graphite platelets in vinyl ester matrix showed approx. 10% better energy absorption than reference E-glass face sheet; whereas the FOE treated T-700 carbon fabric displayed lowest energy absorption. Maximum improvement (about 40%) in energy absorption was observed with Owens Corning HP ShieldStrand® glass fabric face sheets compared to the E-glass/vinyl ester [Figure 15].
Sandwich composites made with five-ply E-glass face sheets and light-weight cores: The third set of low velocity punch-shear tests showed that PVC and Balsa sandwiches absorbed more or less same energy. The Tycor® sandwich composite has glass fiber webs embedded in the foam core. The punch-shear energy absorption at the intersection of the webs was observed to be double of that at foam-region. The response at web line was an average of that at other two locations. Spatial non-uniformity of the core resulted in larger data scatter, with the average response of Tycor® sandwich composite similar to that of PVC foam and balsa wood sandwich composites. EcoCore® sandwich composites absorbed approximately 85% more energy than Tycor, PVC and Balsa sandwiches. The higher density of EcoCore® core provided significant resistance to plunger penetration during impact which resulted in higher energy absorption than other sandwich composites made with light-weight and softer core [Figure 20].

CONCLUSIONS
Test results show more than 10% improvement in impact energy absorption with addition of 2.5 wt. pct. graphite platelets to pure vinyl ester, whereas addition of nanoclay and 1.25 wt. pct. graphite platelet reinforcements showed
detrimental effect. Owens Corning HP ShieldStrand® glass fabric face sheets showed maximum improvement in energy absorption (about 40%) compared to the E-glass/vinyl ester. Fly-ash based EcoCore® sandwiched in between E-glass/vinyl ester face sheets absorbed about 85% more energy than with Tycor®, Balsa wood and PVC foam cores. Cross section microscopy of the damaged samples is ongoing for a better understanding of the energy absorption mechanisms.

ACKNOWLEDGMENTS

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REFERENCES


OUTPUT FEEDBACK CONTROL OF SMART PROJECTILE FIN BASED ON INTERNAL MODEL PRINCIPLE

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ABSTRACT

In this paper, based on the internal model principle, a discrete-time controller is designed for a smart projectile fin for tracking constant and sinusoidal fin angle commands and rejecting disturbances. The model of the smart fin is identified using experimental data. An internal model is included in the forward path of the closed-loop system. The augmented system including the internal model is stabilized using the state variable feedback by placing poles at selected locations within the unit circle. As the states cannot be measured, a state estimator is designed for synthesis using only fin angle feedback. It is shown that in the closed-loop system, the fin angle asymptotically tracks the command fin angle. Laboratory tests are performed which show that the designed controller accomplishes accurate fin angle tracking.

INTRODUCTION

The use of surface mounted or bonded piezoelectric actuators for shape control of intelligent structures has increased lately due to the low cost and flexibility of the composite piezoelectric actuators. The actuator uses inter-digitated electrodes for poling and subsequent actuation of an internal layer of machined piezoceramic fibers. The fiber sheets are formed from monolithic piezoceramic wafers and conventional computer-controlled wafer-dicing methods. The complete description of the piezoelectric actuator used in this paper can be found in [1]. This piezoelectric actuator has been used in wide ranges of applications including, shape control of composite beams, plates, vibration control of robots [2–8]. In addition to this, it is also used in controlling different types of aircraft structural members such as wings, fins, or rotor blades [9–11]. The design of active controllers using piezoelectric actuators for vibration, force and position control has been considered by various researchers [2, 12–16].

Traditionally, mechanical actuators are used for controlling the fin angle of missiles and projectiles to control the path. These actuators are bulky and slow. This underlines the need for developing more efficient actuation mechanisms. Recently, the development of a smart fin model with a piezoelectric actuator for a projectile has been considered in [17]. The adaptive control for the fin-beam model of [17] is based on a modeling error compensation approach in which lumped uncertainties are estimated using a high-gain observer. For stability in the closed-loop system, this controller requires accurate measurement of the fin angle. The adaptive controller in [18] is based on the inverse feedback linearization technique. However, this controller needs either the state feedback or discontinuous output feedback control for synthesis. An adaptive servoregulator has been developed in [19] but this controller requires the knowledge of the sign of the high-frequency gain and requires tuning of gain during real-time control. Moreover, it cannot guarantee asymptotic tracking of the fin angle if the disturbance torque varies with time. A fuzzy logic controller has been developed in [20] for the control of rotation angle of the smart fin. However, the designer has to develop a number of if-then rules which are not easy to obtain. However, the controllers mentioned above considered only constant fin angle tracking and constant disturbance rejection.

The contribution of this paper lies in the design of a discrete-time internal model based controller for a smart projectile fin. The fin angle is chosen as the controlled variable and objective is to follow constant and sinusoidal reference fin angle trajectories and reject disturbances of similar waveforms.
synthesis, it is assumed that only the fin angle is measured. For the controller design, an internal model of the exosignals (constant and sinusoidal) is introduced in the forward path. A linear model of the smart fin identified using the experimental data is used in this study [21]. Then a sampled data control system is designed by stabilizing the complete system including the internal model. For synthesis using only fin angle feedback, a state estimator is constructed. Interestingly, the proposed controller requires no tuning of gains during real-time implementation and requires only fin angle for feedback. Computer simulations and experimental results are presented, which show that the designed internal model-based discrete time control system successfully tracks both constant and time varying trajectories.

DESCRIPTION OF THE PROJECTILE SMART FIN

A schematic representation of the projectile with a smart fin is shown in Figure 1. The smart fins, which are used to steer the projectile, are deployed as soon as the projectile reaches the apogee. The smart fin consists of a rigid aero shell which rotates about the axis fixed to the projectile as shown in the Figure 2.

The piezoelectric bimorph actuator is completely enclosed within the shell. The actuator is composed of two Macro Fiber Composites (MFC’s) [22]. These are supported by gluing them to fiberglass frame at either end of the actuator to mount it within the fin aero-shell. The resulting actuator is shown in Figure 3. Figure 4 shows the placement of the actuator within the aero-shell.

The choice of configuration shown in Figure 2 minimizes the volume and weight of the unit. The piezoelectric bimorph produces strain as voltage is applied to it. One MFC is activated in tension by applying positive voltage (along the fiber axis) while other MFC is activated in compression by applying negative voltage (against the fiber axis). The tensile and compressive strains induce a distributed couple that causes the actuator to bend and rotate the fin at the same time. The fin can be rotated in the opposite direction by changing the polarity of the voltage.

SMART FIN MODEL IDENTIFICATION

The identification of the plant model through the experimental data takes care of the unmodeled dynamics, like friction between the axle and the encoder or actuator and the pin joint etc. as shown in the Figure 2. Moreover, the identified model is amenable to rigorous mathematical analysis. The model of the smart fin is identified by exciting the system with logarithmic sweep chirp signal [23] and measuring the fin angle. When compared to other types of the chirp signals, logarithmic sweep generates large frequencies starting form a low frequency within a relatively short time. The excitation signal selected is of the form:

\[ y_{\text{chirp}} = A \cos(\psi(t) + \phi_0) \]

\[ \psi(t) = A 2\pi f_t \int_0^t f_0 \frac{d(t-\tau)}{f_0} dt \]  

(1)
Table 1: CHARACTERISTICS OF THE EXCITATION SIGNAL

<table>
<thead>
<tr>
<th>Variable</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A$ (scale factor, Volt)</td>
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</tr>
<tr>
<td>$\phi_0$ (initial phase, Rad)</td>
<td>0.0</td>
</tr>
<tr>
<td>$t_g$ (target time, sec)</td>
<td>335</td>
</tr>
<tr>
<td>$f_0$ (initial frequency, Hz)</td>
<td>0.003</td>
</tr>
<tr>
<td>$f(t_g)$ (target frequency, Hz)</td>
<td>100</td>
</tr>
</tbody>
</table>

The values of the parameters used in the Equation 1 are shown in Table 1. The selected excitation signal and the fin angle responses (in degrees) are shown in Figures 5 and 6, respectively.

It is decided to avoid the complexities of creating the nonlinear model that can accurately represent the fin. Instead, a linear model that best fits the input and output data is used. Using MATLAB system identification toolbox [23], the identified third order linear model of the smart fin is given by:

$$\theta(s) = \frac{3.355s + 42.0717}{s^3 + 12.71s + 1334s + 6656}$$  \hspace{1cm} (2)

where, $s$ is the Laplace variable, $\theta(s)$ is the fin angle in degree, and $V_e(s)$ is an effective voltage in volts, which is absolute sum of two individual voltages $V_1$ and $V_2$. $V_1$ and $V_2$ are the voltages applied to two individual MFC actuators. The same input signal of Equation 1 is fed into the Equation 2 and the resulting output of the simulation is compared to the actual output as shown in the Figure 7. The variation in the results can be explained by the nonlinear nature of the MFC actuator. With the advent of digital computers and availability at lower cost, the use of digital control system is very common. Also the ease of integration with physical systems emphasizes the need for digital controller design. The discrete model of the smart fin obtained from Equation 2 with sampling time $T = 0.01sec$ is given by:

$$\theta(z) = \frac{0.0001658z^2 + 1.939 \times 10^{-5}z - 0.0001462}{z^3 - 2.754z^2 + 2.64z - 0.8806}$$ \hspace{1cm} (3)

The zero/pole/gain representation of Equation 3 can be written:

$$\theta(z) = \frac{1.658 \times 10^{-4}(z + 0.9991)(z - 0.8821)}{(z - 0.9499)(z - 0.9499 + 0.3372i)(z - 0.9499 - 0.3372i)}$$ \hspace{1cm} (4)
Equation 3 can be represented in a state-space form as:

\[
X((k+1)T) = AX(kT) + Bu(kT)
\]

\[
y(kT) = CX(kT)
\]  

(5)

The system matrices are

\[
A = \begin{bmatrix}
2.754 & 1 & 0 \\
-2.640 & 0 & 1 \\
0.880 & 0 & 0
\end{bmatrix},
\]

\[
B = \begin{bmatrix}
1.658 \times 10^{-4} & 1.939 \times 10^{-5} & -1.462 \times 10^{-4}
\end{bmatrix}^T,
\]

\[
C = \begin{bmatrix}
1 & 0 & 0
\end{bmatrix}
\]

where \(X(kT) \in \mathbb{R}^3\), is the state vector, \(u(kT) = V_e(kT)\), the input and \(y(kT) = \theta(s)\) is the output variable. Suppose, \(r(kT)\) is a given reference fin angle trajectory. We are interested in designing a robust internal model-based control law such that, the fin angle, \(y(kT)\) asymptotically tracks the reference fin angle, \(r(kT)\). For simplicity, the argument \(T\) is omitted hereafter.

**ROBUST TRACKING USING INTERNAL MODEL PRINCIPLE**

Internal model principle states that, a signal can be tracked or rejected provided that a servo compensator (internal model of exosignals) is inside the control loop [24], [25]. The block diagram of the controller with the internal model and the state feedback stabilizer is shown in the Figure 8.

**TRACKING CONSTANT REFERENCE COMMAND**

Disturbance rejection and tracking of the constant command signals can be achieved by introducing a new state variable \(x_a\) that integrates the difference between the command input \(r(k)\) and output \(y(k)\) [26] as shown in the Figure 9. The augmented plant is represented as:

\[
\begin{bmatrix}
X((k+1)) \\
x_a(k+1)
\end{bmatrix} = \begin{bmatrix}
A & 0 \\
-C & 1
\end{bmatrix} \begin{bmatrix}
X(k) \\
x_a(k)
\end{bmatrix} + \begin{bmatrix}
B \\
0
\end{bmatrix} u(k) + \begin{bmatrix}
0 \\
r(k)
\end{bmatrix}
\]  

(6)

The control law is taken of the form:

\[
u(kT) = [-K -K_a] \begin{bmatrix}
X(k) \\
x_a(k)
\end{bmatrix}
\]  

(7)

Using Equations 6 and 7, the closed-loop system is represented as:

\[
\begin{bmatrix}
X(k+1) \\
x_a(k+1)
\end{bmatrix} = \begin{bmatrix}
A - BK -BK_a & -C \\
0 & 1
\end{bmatrix} \begin{bmatrix}
X(k) \\
x_a(k)
\end{bmatrix} + \begin{bmatrix}
0 \\
r(k)
\end{bmatrix}
\]  

(8)

The gains \(K \in \mathbb{R}^3\) and \(K_a \in \mathbb{R}\) are found by placing the closed loop poles at the desired locations inside the unit circle.

**TRACKING SINUSOIDAL REFERENCE TRAJECTORY**

The reference and disturbance of sinusoidal nature can be successfully tracked and rejected, respectively, by using the internal model of of the similar frequency. The internal model selected is given by:

\[
\frac{1}{z^2 - 2\zeta \omega T + 1}
\]  

(9)

Internal model is introduced in the forward path of the closed loop system using the state variables \(x_{1a}\) and \(x_{2a}\) as shown in the...
Figure 10. The augmented system with internal model can be represented as:

\[
\begin{bmatrix}
X(k+1) \\
x_{1a}(k+1) \\
x_{2a}(k+1)
\end{bmatrix} =
\begin{bmatrix}
A & 0 & 0 \\
0 & 2\cos(\omega T) & 1 \\
-C & -1 & 0
\end{bmatrix}
\begin{bmatrix}
X(k) \\
x_{1a}(k) \\
x_{2a}(k)
\end{bmatrix} +
\begin{bmatrix}
B \\
0 \\
0
\end{bmatrix} u(k) +
\begin{bmatrix}
0 \\
0 \\
r(k)
\end{bmatrix}
\] (10)

The closed loop system is stabilized using a control law of the form:

\[
u(k) = [-K - K_{1a} - K_{2a}]
\begin{bmatrix}
X(k) \\
x_{1a}(k) \\
x_{2a}(k)
\end{bmatrix}
\] (11)

The gains \( K \in \mathbb{R}^3, K_{1a} \in \mathbb{R} \) and \( K_{2a} \in \mathbb{R} \) are found by placing the closed loop poles at the desired locations inside the unit circle. The closed loop system with control law of Equation 11 is given by

\[
\begin{bmatrix}
X(k+1) \\
x_{1a}(k+1) \\
x_{2a}(k+1)
\end{bmatrix} =
\begin{bmatrix}
A-BK_{1a} & -BK_{2a} & -BK_{2a} \\
0 & 2\cos(\omega T) & 1 \\
-C & -1 & 0
\end{bmatrix}
\begin{bmatrix}
X(k) \\
x_{1a}(k) \\
x_{2a}(k)
\end{bmatrix} +
\begin{bmatrix}
0 \\
0 \\
r(k)
\end{bmatrix}
\] (12)

**STATE ESTIMATOR**

The state feedback mentioned in the previous section can be implemented only when the states can be measured without error. As the states do not represent any physical quantity, direct measurement of the states is not possible. To address the issue of state measurement, an observer is designed to estimate the states using the input and output of the plant [26]. Block diagram of the closed loop system with the internal model and the state estimator is shown in Figure 11. Let \( q(k) \in \mathbb{R}^3 \) be the estimated states using the plant input, \( u(k) \), and output, \( y(k) \). The observer is taken of the form,

\[
q(k+1) = Aq(k) + Bu(k) + L(y(k) - Cq(k))
\] (13)

Subtracting the Equation 13 from Equation 5, the governing equation for estimation error can be written as:

\[
e(k+1) = (A - LC)e(k)
\] (14)

The gain vector, \( L \in \mathbb{R}^3 \) is chosen such that \( (A - LC) \in \mathbb{R}^{3 \times 3} \) has all eigenvalues within the unit disk at desired locations. Usually, estimator poles are taken 5 to 10 times faster than the closed-loop poles.

**DIGITAL SIMULATION RESULTS**

The simulations results for the smart fin based on the identifies model (Equation 3) are presented in this section. MATLAB/SIMULINK tools are used to simulate the dynamics of the smart fin system.

**TRACKING CONSTANT COMMAND**

The state feedback gains of the smart fin model including the first-order internal model are obtained by placing the poles of the augmented system (Equation 8) at \( P_e = [0.9 \ 0.8 + 0.2i \ 0.8 - 0.2i \ 0.87] \). The closed-loop poles are selected in such a way that control input is within the limits. The state feedback gains corresponding to the desired pole locations are

\[
K = [-1.8912 \ -9.4953 \ -16.278] \times 10^3
\]

\[_{\text{are}}
\]

\[
K_{1a} = -.20485 \times 10^3
\]

The estimator gains are obtained by placing the poles at \( P_e = [.02 \ .3 \ .4] \) are

\[
L = [2.0060 \ -2.5850 \ .91440]
\]

Figure 12 shows the simulation results for fin angle command of 3 deg. It is observed that the fin angle asymptotically converges to the desired value within 0.5 sec. The effective control input needed for the fin to deflect to an angle \( \theta = 3 \) deg is around 400 V.

**TRACKING SINUSOIDAL COMMAND**

Tracking of the sinusoidal command signal is done by stabilizing the augmented system given in Equation 12 by placing the closed-loop poles at \( P_e = [0.9 \ 0.85 + 0.2i \ 0.85 - 0.2i \ 0.95 \ 0.92] \). The obtained gains are

\[
K = [3.6767 \ 3.2755 \ 2.6625] \times 10^3
\]

\[
K_{1a} = -24.925
\]

\[
K_{2a} = -24.333
\]

---

Figure 11: Internal model based smart fin control with state estimator
Figure 12: Simulation results for tracking constant command of 3 deg

The designed controller is tested for fin angle command of 2 deg and frequencies 0.2 Hz and 0.5 Hz. Figure 13 shows the tracking of the 2 deg fin angle at 0.2 Hz frequency. It is observed that the fin angle tracks the command input with zero error. Control input required is around 300 volts. Figure 14 shows the tracking of the 2 deg fin angle at 0.5 Hz frequency.

Figure 13: Simulation results for tracking command fin angle of 2 deg and 0.2Hz

Figure 14: Simulation results for tracking command fin angle of 2 deg and 0.5Hz

EXPERIMENTAL RESULTS

A prototype of the smart fin is developed, as shown in Figures 2 and 15, in the laboratory for real-time tests. The shell of the fin is created using a rapid prototyping machine. It has a NACA0026 profile with a chord length and a span of 177.8 mm and 106.7 mm, respectively. Two MFCs (Model No. M8557P1 – 5H2, Smart Material) [22] are bonded using adhesive epoxy (3Ms DP 460 Epoxy), having glass fiber at either end of the MFCs in order to have a chance for mounting in the experimental setup. The MFC can operate between -500 V to +1500 V. Two differential amplifiers, which can supply -1000 V to +1000 V, are used to apply the voltages to MFC’s. Due to symmetry, V2 is set to be equal to -V1. A through-shaft incremental encoder, (15T – 05SB – 2500N5QHV – F03, Encoder Product Co.), is used to measure the rotation angle of the smart fin. This encoder requires external hardware to setup home position of the smart fin. The encoder gives a quadrature signal with 2500 counts of pulses per revolution, which gives an angular measurement resolution of 0.036 degree. The real-time control software (Quanser WINCON4.1, Multi – Q3 Terminal board) is used to control the smart fin. The layout of the experiment is shown in Figure 16.

The numerical simulation results in the previous section show that controller asymptotically tracks both constant and time varying commands with zero steady state error. To verify the ap-
The applicability of controller, experiments are conducted on the prototype of the smart fin as described above. Figure 17 shows the experimental results for tracking the command fin angle of 3 deg. Considering the nonlinear nature of the smart fin and the identified model being linear, transient nature of the smart fin in real-time control differs from that of the digital simulations. In addition to this, as shown in Figure 15, the smart fin consists of many mechanical interconnected elements which may induce considerable amount of friction. It is observed in Figure 17 that smart fin tracks the 3 deg fin angle with zero steady-state error. The control input is higher in real-time experiment due to the reasons stated above.

CONCLUSIONS

This paper considered fin angle control of a smart projectile fin using the piezoelectric bimorph actuator. A discrete-time
model of the smart fin was identified using the experimental data. An internal model based control system was designed for tracking and rejecting constant and time varying fin angle trajectories. The state variables were estimated by observing the input, effective voltage and output, fin angle of the plant. Simulation results showed that the designed internal model based controller can successfully track the command fin angles. Experiments were conducted using a prototype of the smart fin. The computed feedback and estimator gains were used in the experiments without any modifications. Experimental results showed that the proposed controller can successfully track the constant fin angle of 3 deg with zero steady-state error. Sinusoidal trajectories were tracked with error depending on the frequency of the command fin angle.

REFERENCES


MODELING OF FLUID FLOW IN CORTICAL BONE

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ABSTRACT
Understanding fluid flow in bones is a critical element in understanding nutrient and waste transport, bone mechanotransduction, and bone loss in microgravity. The constitutive relations of the poroelasticity theory are employed and it is assumed that both the whole bone and its characteristic substructure, the osteon, may be modeled as porous hollow cylinders that allow fluid flow only through their inner boundaries. Based on the solution of the unconfined compression boundary value problem, an experiment is built to measure the permeability in the micron-level of the lacunar canalicular porosity (PLC) of the bone. These results allow the creation of a theoretical model for fluid flow in a nested hierarchical system of porosity levels, where the lowest level porosity, the PLC, is considered to be a point source of fluid in the higher level vascular porosity (PV). The results suggest that the influence of the PV pore pressure on the PLC pore pressure is very small (less than 3%) and a hierarchical model is more architecturally precise in modeling porosity structure than the dual porosity models that have been suggested. The results give insight into nutrition and waste transport in bones.

INTRODUCTION
This paper presents a theory for the poroelasticity for porous materials with a special type of pore space structure. This particular pore space structure model is developed as a model for interstitial pore fluid flow in tissues like bone, tendon, meniscus and possibly other tissue types. The special type of pore space structure is described as “Nested Porosity” because a particular pore size porosity can only drain its fluid into, and receive its fluid supply from, a nearest neighbor porosity, a “nearest neighbor” in terms of the pore size of its porosity. These different pore size porosities are nested within the other pore size porosities like a nested set of Russian dolls; the nesting or ordering criterion is the porosity pore size. The nested porosities are connected so the pore fluid may flow easily through each and across the boundaries between the two nearest neighbor porosities, but any particular pore size porosity may only interchange its pore fluid with the next larger pore size porosity and the next smaller pore size porosity. In modeling a nested poroelastic material the pore fluid pressure is distinct in each one of the nested porosities. The boundaries of a representative volume element (RVE) for a continuum model may be established for each of the nested pore size porosities. If the interstitial bone fluid flow is unidirectional in a nested system, as it is in the vascular system, the flow from pore size porosity into another is also unidirectional. The pore sizes in cortical bone are approximately three discrete sizes; the largest pore size (approximately 50 μm diameter) is associated with the vascular porosity (PV), the second largest pore size (approximately 0.3 μm diameter) with the canaliculi in the lacunar-canalicular porosity (PLC) and the smallest pore size (approximately 10 nm diameter) is in collagen-apatite porosity (PCA) but is not of interest in the present study. The pore fluid pressure in these two pore size porosities is also quite different. Under physiologically possible rapid rise-time loadings of bone, the pore fluid pressure may rise considerably in the PLC [1]. The decay time for this pore pressure rise is much larger in the PLC than it is in the PV. The PV is a low-pore-fluid-pressure domain because the PV permeability is sufficiently large to remit a rapid decay of a pressure pulse. This must be the case because the PV contains thin walled blood vessels carrying blood with a pressure of 40 to 60 mm of Hg. Figure 1 shows the details of these two porosities.
THE UNCONFINED COMPRESSION TEST OF A POROUS DISK

The problem of confined and unconfined compression tests of porous disks compressed between two parallel rigid and impermeable smooth plates has been under investigation by many authors in the past few decades. The impermeable plates would allow flow only in the radial direction in the unconfined compression experiment as shown in Figure 2 on the right. On the other hand, in a confined compression experiment the fluid exudation in the (z) direction is shown in Figure 1 on the left. In the unconfined compression test, either a step in end plate displacement may be applied, which would constitute a stress relaxation test, or a step in total applied end force load may be applied, which would constitute a creep test. In unconfined compression, the contact with the plates is assumed to be totally frictionless, so the deformation might be expected to be independent of (z); thus this axisymmetric problem becomes a one-dimensional problem in the radius and fluid flow will occur in the radial direction. The unconfined compression test was used to study the mechanical behavior and load effects of hydrated soft tissues such as articular cartilage [2], growth plate and chondroepiphysis [3], where an incompressible transverse isotropic model was presented. The problem was solved with the assumption of compressibility of the fluid and the matrix [4], and the solution is extended to annular porous disks in [5], where 3 sets of boundary conditions were investigated. The first set of boundary conditions allows fluid passage from both the outer and the inner cylindrical boundaries of the annular cylinder. The second set of boundary conditions allows free fluid passage from the outer boundary and none across the inner boundary. The third set of boundary conditions seal the outer boundary and allow free fluid passage from the inner boundary. An illustration of the experimental test situation is shown in Figure 2. The symmetry of the unconfined compression problem suggests that it is reasonable to assume that the displacement and pressure fields are axisymmetric. The compressive strain in the axial direction is homogeneous, a condition only obtainable if the two impervious plates are perfectly frictionless. A direct result on the kinematics of deformation is that all stresses and strains are independent of (z). Therefore the (r,z) axes are principal axes. Thus there are no shear strains and hence no shear stresses exist on these coordinate planes. Three constitutive relations from the theory of poroelasticity include stress-strain-pore pressure relation, the fluid content-stress-pore pressure, and Darcy’s law were used to solve this boundary value problem [5].

THE POROELASTIC PROPERTIES OF THE PLC

The osteon is composed of a central Haversian canal housing a blood vessel and is surrounded by alternating mineralized collagen lamellae. The mean Haversian canal and osteon radius estimated roughly to be 100–150μm respectively [6]. Their small size and stiffness make osteons challenging to isolate, nonetheless several approaches have been described in the literature. Ascenzi, [7] and [8], developed a method for extraction of osteons from a thin cross-section of bone using a sharp steel needle eccentrically inserted in a dentist’s drill or using a custom made micro lathe. Osteons have also been isolated by propagating a fracture through the natural boundary of the osteon, [9], and using a precision and computer controlled osteon push-out micro-testing system [10]. Most osteons in cortical bone do not have a perfectly cylindrical shape; however, for their testing and analysis, osteon samples were prepared into cylindrical shaped specimens in a recent approach, [11], that suggested using Micro-CT imaging and Micro-lathe to extract the osteons. An image generated in the Micro-CT is shown in Figure 3.
Figure 3: Micro-CT image of an isolated osteon. The image shows the three main views and the Haversian canal which can be measured from these images.

A miniature uniaxial material testing stage was developed by our group for the assessment of mechanical properties in small bone samples. The computer controlled stage comprises an Intelligent Picomotor control module (8753 driver, New Focus Inc.) and an Ethernet controller (8752 Ethernet controller, New Focus Inc.). The driver was connected to a small piezoelectric motor (Picomotor, New Focus Inc.) which has a displacement resolution of 30 nm. The Z-stage held a stainless steel platen vertically aligned to a second platen in a loading chamber filled with water, and connected to a load cell (GS series gram force - 10 grams- sensor, Transducer Technique Inc.). The resolution of the measurement was 0.05% (5 mg) of the load cell’s full scale. Load cell output signal was amplified using an instrumentation amplifier (INA 122, Texas Instruments) and then calibrated using standard weights to display the measured force in grams. Voltages were converted into digital signals using a data acquisition interface (USB6810, National Instruments) and visualized in real time using LabView (V8.5, National Instruments). A schematic diagram for the loading system is shown in Figure 11.

In order to perform a stress relaxation test in the sample, the loading stage was used under displacement control. The user inputs the desired strain rate in LabView, along with the type of test (compression or tension), then sends the commands to the Ethernet controller and the picomotor stage. The loading system performance was tested using a cylindrical steel sample in stress relaxation test [12]. The osteon specimen was pre-stressed with 0.2g and then loaded using a constant strain rate $\dot{\varepsilon}_p$ for a period of time $t_0$ during which the applied strain was rising linearly from a value of 0 to 2 g of force approximately. After time $t_0$ the value of $\varepsilon(t)$ was held constant. The loading system is shown in Figure 4. The sample was left to freely undergo relaxation until the change in measured force was no longer significant. The load vs. time curve was displayed in real time on the screen and stored in the hard drive for curve fitting to the analytical solution that was developed previously [5]. Figure 4 shows the development of the loading system which is computer-controlled via a network driver controller using a custom LabView application.

Figure 4: A uniaxial micro-mechanical testing device was constructed based on a small piezoelectric motor. The motor was integrated to a custom compression loading stage, and axially aligned to a load cell, [11].

The intrinsic permeability was obtained by curve fitting the theoretical model, [5], to the experimental stress relaxation time history using the least-squares algorithm. The results showed that the radial permeability is in the range of $10^{-24} – 10^{-23}$ m$^2$, [11]. The drained poroelastic properties have shown good agreement with the previously reported.

THE POROELASTIC MODEL OF THE OSTEON OR PLC

Using the hierarchical scheme described in [13], a model is formulated in this section for the transport of bone interstitial fluid between the PV and PLC porosity levels in osteonal cortical bone. A section of this bone is illustrated in Figure 1. In this paper the PV and the PLC will both be modeled as poroelastic hollow circular cylinders. The poroelastic hollow circular cylinder model of the PLC connects through its inner cylindrical wall to the PV; the hollow part of this cylinder is actually part of the PV. The inner surface of the cylinder representing the PLC is the surface across which the two porosities exchange pore fluids. The PLC is assumed to permit flow across its inner radial boundary, but not its outer radial boundary. While other assumptions are possible, an earlier study [14] showed that this is a reasonable assumption. The PV is assumed to permit flow across both of its radial boundaries. The PLC hollow cylinder is the osteon of Figure 1. The PV
hollow cylinder is the entire bone of Figure 1 with central lumen of the whole bone, the medullary canal, constituting the hollow part of the PV model. Both of these models are continuum models and the transport connection between the two continua is the outflow-influx that occurs across the osteonal or Volkmann inner wall between the PLC and the PV [15]. In the domain between the inner surface and outer surface of the PV cylinder there are area sources-sinks that permit interchange of fluid between the two continuum models representing the PV and the PLC.

The pressure distribution in the PLC can be rewritten from [3] and [5]

\[
\frac{\partial^2 p^i}{\partial \lambda^2} + \frac{1}{\lambda} \frac{\partial p^i}{\partial \lambda} - \frac{\partial^2 p^i}{\partial t^2} - \frac{b^2}{b^2} \frac{\partial p^i}{\partial t} = \frac{\mu b^2}{k_p} \left( A \frac{\partial \dot{e}}{\partial t} + A \frac{\partial f(t)}{\partial t} \right), \tag{1}
\]

where \( p \) is the pore pressure, \( \lambda \) is the non dimensional radius of the PLC, \( t \) is the time, \( A_r \) and \( A_z \) are Biot’s effective stress coefficients, \( k_p \) is the radial permeability, \( \dot{e} \) is the strain rate, \( c \) and \( f(t) \) are constants, \( \mu \) is the viscosity, \( b \) is the outer radius, and the superscript \( L \) refers to the PLC. Notice that \( p \) is a function of \( \lambda \) and \( t \).

Three conditions were considered, thus

\[
\begin{align*}
(\text{i}) & \quad p^i(\lambda,0) = 0, \\
(\text{ii}) & \quad p^i(a,t) = p^i(\beta,t), \\
(\text{iii}) & \quad \frac{\partial p^i(1,t)}{\partial \lambda} = 0, \tag{2}
\end{align*}
\]

where \( \beta \) is the non dimensional radius of the PV, \( a \) is the non dimensional inner radius of the PLC, and the superscript \( V \) refers to the PV. The second condition shows that the Haversian canal in the PLC is influenced by the PV pore pressure. Our aim here is to solve Eq.(1) for a ramp loading in stress relaxation test. Eq.(1) is a non homogenous equation with non homogenous boundary conditions, thus we applied Duhamel’s integral to solve this type of problems by having an auxiliary function that will yield a Sturm –Liouville problem. Thus the solution for a rising displacement is

\[
p^i(\lambda,t) = p^i(\beta,t) - N^i \varepsilon(t) + \sum_{\nu=1}^{\infty} C \left( A \frac{\partial \dot{e}^i}{\partial t} + A \frac{\partial f(t)}{\partial t} \right) \frac{k_p^2 c^2}{b^2} e^{-\frac{k^2 \lambda^2}{b^2}}.
\]

\[
M^i \left\{ \int_0^\lambda e^{\frac{k^2 \lambda^2}{b^2}} \frac{\partial p^i}{\partial \tau} \, d\tau \right\} + N^i \left\{ \int_0^\lambda e^{\frac{k^2 \lambda^2}{b^2}} \varepsilon(\tau) d\tau \right\}.
\]

Ignoring the first term and the first integral in the right hand side yields a condition where the PV has no influence over the PLC.

The outflow /influx between the PLC level and the PV level will be calculated directly from the pore fluid pressure gradient at the osteonal wall of the PLC level, hence the fluid flow \( \gamma \) in unit density/sec integrated over a unit length is recorded here as

\[
\gamma^i = \frac{1}{b a_{cl}} \frac{1}{k_p} \frac{\partial p^i}{\partial \lambda}, \tag{4}
\]

where \( a_{cl} \) denotes the area of an osteon inside the cement line. If the PV pressure effects on the PLC are ignored then the PLC pore pressure distribution can be plotted as shown in Figure 5.

![Figure 5: The flow across the non dimensional radial distance in a ramp loading at different rising times.](image)

The material properties for the PV and the PLC are shown in Table 1, where the superscripts \( m \) and \( d \) stands for drained condition and matrix material.

**THE NESTED TWO-PORE-SIZE-POROSITY MODEL FOR INTERSTITIAL FLOW IN CORTICAL BONE TISSUE**

The nested two-pore-size-porosity model for interstitial flow in cortical bone tissue is described here using Figure 6 and the properties of the anatomical structures described in the text above.

To fix notation we introduce two cylindrical coordinate systems, one centered in the typical osteon in Figure 1 and one centered on the idealized whole bone cross-section in the same figure in the center of the medullary canal. For the larger idealized bone cross-section we assign the notation \( (R, \vartheta, Z) \) to the cylindrical coordinate system and for the smaller osteonal coordinate system we assign the notation \( (r, \theta, z) \) to the cylindrical coordinate system. Further, we consider the annular cross-section of a long bone in Figure 1 to be subjected to an axial stress \( \sigma(r, \theta, t) \), which is a function of location on the cross-section \( (r, \theta, z) \) and time \( t \). This means that for an osteon whose center is located at \( (R, \vartheta, Z) \) in the cross-section is subjected to \( \sigma^*(r^*, \theta^*, t) \) which is assumed to be uniform over the cross-section of that particular osteon, the values of \( r^* \) and \( \theta^* \) serving to identify that osteon.
Table 1: Properties of the PV and PLC, Cowin et al. (2009)

<table>
<thead>
<tr>
<th>Material Parameters</th>
<th>PLC (L)</th>
<th>PV (V)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$E_1^d = E_1^d$</td>
<td>15.17 GPA</td>
<td>12.7 GPA</td>
</tr>
<tr>
<td>$E_3^d$</td>
<td>15.96 GPA</td>
<td>14.9 GPA</td>
</tr>
<tr>
<td>$V_{12}^d = V_{21}^d$</td>
<td>0.316</td>
<td>0.27</td>
</tr>
<tr>
<td>$V_{31}^d = V_{32}^d$</td>
<td>0.308</td>
<td>0.285</td>
</tr>
<tr>
<td>$V_{13}^d = V_{23}^d$</td>
<td>0.282</td>
<td>0.27</td>
</tr>
<tr>
<td>$E_1^m = E_1^m$</td>
<td>18.6 GPA</td>
<td>18.6 GPA</td>
</tr>
<tr>
<td>$E_3^m$</td>
<td>22.32 GPA</td>
<td>22.32 GPA</td>
</tr>
<tr>
<td>$V_{12}^m = V_{21}^m$</td>
<td>0.322</td>
<td>0.322</td>
</tr>
<tr>
<td>$V_{31}^m = V_{32}^m$</td>
<td>0.312</td>
<td>0.312</td>
</tr>
<tr>
<td>$V_{13}^m = V_{23}^m$</td>
<td>0.255</td>
<td>0.255</td>
</tr>
<tr>
<td>The Outer Radius $R_o = 160 \mu m$</td>
<td>$R_o = 0.03 m$</td>
<td></td>
</tr>
<tr>
<td>The Inner Radius $R_i = 32 \mu m$</td>
<td>$R_i = 0.015 m$</td>
<td></td>
</tr>
<tr>
<td>The Porosity $\phi$</td>
<td>0.05</td>
<td>0.05</td>
</tr>
<tr>
<td>the permeability $k_{xx}$</td>
<td>$2.2 \times 10^{-24} m^2$</td>
<td>$6.3 \times 10^{-10} m^2$</td>
</tr>
</tbody>
</table>

Thus, $p^e$ satisfies the condition of impermeability at the cement line and equality with $p^f$ at the wall of the osteonal canal.

Based on all the previous results two conditions can be imposed on the pressure in the PV. The first one implies no flow through the periosteum, the outer boundary, and the second one stems from the fact that the PV is a low-pore-fluid-pressure domain because it contains thin-walled blood vessels carrying blood with pressure of 40 to 60 mm of Hg; a pore fluid pressure significantly greater than 40 to 60 mm of Hg will collapse these blood vessels. Therefore, it will be important to assume that the pressure on the endosteum walls (the inner boundary) is a low pressure, but not zero. This low pressure allows flow through the inner boundaries of the PV. So one can assume the following conditions

$$p^e (A, t) = p^{bo} \sin wt, \quad \frac{\partial p^e (1, t)}{\partial \beta} = 0, \quad p^e (\beta, 0) = 0 \quad (5)$$

where $A$ is the non dimensional inner radius of the PV, $p^{bo}$ is the blood pressure, should not exceed 60 mm Hg, and $w$ is derived from the frequency of the pulses (72/s) in rad/s. The partial differential equation for pore pressure in the PV should be the same as for the PLC, Eq.(1), but with only one difference, that is adding a source term for fluid flow, Eq.(4), from the PLC which acts as a point source for fluid. Thus the pressure distribution in the PV can be expressed in terms of the PLC pore pressure which indicates the coupling of the two porous systems. The PV pore pressure distribution is illustrated in Figure 7, which shows clearly that the pore pressure in the PV is maintained low along the walls of the endosteum or the medullary canal.

DISCUSSION

The long term objective of the work, of which this paper is a part, is to develop a model of all fluid transport in bone, particularly that due to mechanical loading and blood pressure. The result presented here is the basic piece of this model. It addresses the question of pore fluid movement from the perivascular region in bone to the bone cells housed in the...
lacunae of the mineralized matrix. Knowledge of this fluid movement is necessary for the determination of the nutrient transport and the effect of the fluid drag on the cell processes of osteocytes in the canaliculi, which is thought to be a principal mechanotransduction mechanism. Quantification of the fluid drag on the cell processes is necessary for the evaluation of osteocytes mechanosensitivity [16] [17].

Another motivation of this study is to understand how the PV pressure influences the PLC pore pressure, Figure 8, which could be deduced from Eq. (3) by neglecting or including the first term and the first integral in the right hand side, in other words including or excluding the PV effects. The results which are shown in Figure 8 show that the influence is very little, less than 3%, which supports the basic fact that the PV is a low pressure reservoir and its pore pressure can not exceed certain limits. Thus, future in vitro experiments can evaluate this influence.

The fluid flow into the Haversian canal is expected to be affected by this pore pressure variation. Thus Eq.(4) describes the two scenarios, with and without the PV effect. The presence of a pressure in the inner walls of the osteonal canal should reduce the fluid flow (quantitatively). When looking at this scenario we found that the decrease in the volume of fluid flowing into the Haversian canal is very small also, less than 6%. Inclusion of the blood pressure when doing in vitro experiments will be an interesting area of research. The advantage of this analysis is that it extends to hard tissues, through the lack of the incompressibility assumption and the annular disk shape, an analytical model for an experimental test situation. Thus, the poroelastic material properties and the permeability for the PV and PLC could be determined through the experimental testing combined with the presented analytical model [11]. The advantage will be to determine the PV permeability with inclusion of the nested porosity, the PLC. This permits a more detailed study for bone porosity and the nested system of lacunar-canalicular porosity (PLC) and vascular porosity (PV) in long bones where these different boundary conditions will give an insight into the nature and quantity of the flow between these porosities. The analysis deviates from the assumption of incompressible constituents which is mostly used in biomechanics. The poroelastic community is aware of the Skempton parameter, a parameter that has a range from zero to one and represents the fraction of the hydrostatic component of the stress in the matrix material that is mechanically transferred to the fluid pore pressure. In effect the pore pressure is shielded from the matrix material hydrostatic stress by the much greater bulk compressibility of the matrix material [5].

![Figure 7: The effect of the PV pressure on the PLC pressure. The figure shows clearly that the PV pressure has small effect on the PLC pressure.](image1)

![Figure 8: The volumetric flow in density/sec when t = 0.4 seconds. Notice that the flow across the cement line is zero.](image2)

On the other hand the PV flow through the medullary canal, the maximum, can be calculated as well. This flow is contributed by the PV and the point sources, the PLC. Figure 9 shows the flow through the medullary canal in a ramp loading. The flow is characterized by a fast rising and a gradual decrease. This will give an insight into the nutrients and waste transport in bone tissues.
REFERENCES


ABSTRACT

Force-measuring platforms are used to study the postural sway of individuals in an attempt to identify balance problems and predict falls in the elderly. Newer non-linear analyses, such as fractal analysis, have shown promise in indicating underlying differences in postural sway patterns based on health and disease that could be keys to achieving such goals and better characterizing postural control.

This paper examines the novel finding of two unique scaling regions observed in the Detrended Fluctuation Analysis (DFA) plots of 60 second quiet-standing postural sway data during a study to determine differences between older adult fallers and non-fallers. The presence of two regions suggests a more complex postural control system than previously thought, utilizing both open-loop and closed-loop feedback.

INTRODUCTION

Measurement of postural stability has the potential to identify underlying balance deficits in patients, but its clinical utility has been limited by uncertainty as to which sway characteristics are most insightful [1,2]. Recent work has suggested that fractal analysis methods, which examine the underlying trends of signals, are more powerful than traditional methods for characterizing postural sway patterns [3,4,5]. If sway can be better characterized it would allow for improved clinical diagnosis.

Postural instability is one of the major risk factors leading to falls in older adults [6]. It is also a hallmark of many pathological conditions, including Parkinson’s disease [7]. As such, it is important to measure the degree of postural instability an individual exhibits in an effort to determine whether abnormality exists. When postural instability is identified, it is often possible to implement interventions to lessen the effect and increase quality of life [7,8]. For example, older adults who exhibit increased postural instability that puts them at high-risk of falling often benefit from a prescribed balance and muscle strengthening program [8].

A common method of measuring the degree of postural instability is static posturography [9]. Static posturography requires subjects to stand on a stationary force-measuring platform, which contains either strain-gage or piezoelectric load transducers [10,11]. As the individual sways due to natural oscillation of his or her center of mass (COM), the ground reaction force is in constant movement attempting to control this dynamic sway [12]. The location of the ground reaction force at the plate surface, known as the center of pressure (COP), is measured by the load transducers in the plate based on the moments and force applied by the feet [11,12]. The COP is recorded separately for the anterior-posterior and medial-lateral directions of sway to best characterize postural sway movement [1]. Though center of pressure displacement is not equivalent to center of mass displacement, it is commonly used as an indicator of the degree of sway because of its high correlation to the COM and the relative ease of measurement under quiet-standing conditions [12,13].

Postural instability is determined by the characteristics of the COP movements. However, there are over fifty separate postural sway parameters that can be calculated from the COP data to describe the degree of stability observed [14]. There is currently no consensus as to which of these parameters are most important to report [1,2]. Traditionally, researchers choose a subset of parameters to examine, most commonly related to the statistical properties of the time-domain data collected, such as the sway range or area [1,15].

Newer analysis methods show promise of revealing more by examining data at a deeper level [5]. Recent developments in non-linear analyses have shown the promise of fractal analysis methods in differentiating healthy from diseased function for a wide range of physiological functions [5,16]. Temporal fractal analysis examines the underlying repeating patterns and trends of time-series data, often revealing more insightful information than traditional statistical calculations [4,5]. These underlying patterns are characterized with a fractal dimension, a numerical value associated with the type of trends observed [17]. This value allows different signals to be compared to each other, with breakdown of the pattern being correlated to a variety of pathological problems [16].

There are a number of related methods that can be used to obtain a fractal dimension [4]. However, there has been much discussion in literature as to which method is most appropriate to use for postural sway data [4,18,19]. Stabilogram Diffusion Analysis (SDA) was the original proposed method to determine...
the fractal dimension of COP [20]. The SDA method revealed that there were two underlying fractal-patterns present in postural sway data, a persistent-pattern for short periods of time of approximately one second and an anti-persistent pattern for longer periods of time [20]. This was a novel finding and allowed researchers and clinicians to gain insight into the probable control of the postural sway system and the use of feedback in its regulation.

The SDA method and the related-findings have been regularly contested [18,19]. Delingeres et al. demonstrated that the presence of the two unique patterns identified by the SDA method were in fact statistical artifacts [18]. The method of SDA assumes the data to be unbounded, however the data is indeed bounded by the dimensions of the feet when standing on the platform, which restrict the movement of the center of pressure to within the base of support [18]. Subsequently, the use of SDA and the interpretation of two patterns of postural control have been cautioned [18]. As an alternative, Detrended Fluctuation Analysis (DFA) has been recommended for analysis of COP data [18]. The DFA method cumulatively sums the data, so that data can correctly be considered unbounded. This results in the presence of only a single pattern, as repeatedly published in literature [4,18,19].

This paper details the DFA findings that were observed during a large-scale study of older fallers and non-fallers in an attempt to determine which traditional and fractal parameters best differentiated the large group. Detrended Fluctuation Analysis was chosen based on the recommendations of literature. In performing DFA calculations for the study, a novel finding was revealed that the DFA plots showed the presence of two unique patterns. This paper aims to examine these findings and what they mean both in regard to postural control and, more generally, the use of fractal analysis methods.

**METHODOLOGY**

*Subjects and Testing Protocol*

One hundred and fifty individuals over the age of 65 participated in this study. Subjects were relatively healthy and independent, all living in the community or in independent living retirement facilities. Subjects were classified as repeat-fallers if they self-reported having fallen at least twice in the year prior to testing. All other subjects were classified as non-repeat fallers. There were 21 repeat fallers (13 female, 8 male; mean age: 83.6 ± 7.6; mean height: 164.3 ± 9.3 cm; mean weight: 72.5 ± 17.5 kg) and 129 non-repeat fallers (97 female, 32 male; mean age: 81.1 ± 7.9; mean height: 163.2 ± 10.5 cm; 72.4 ± 17.4 kg). All subjects gave written informed consent prior to participation.

Subjects performed four quiet-standing trials on the force-measuring platform (Bertec Corporation, Columbus Ohio) in a randomized order: eyes open while standing comfortable (EO-CS); eyes closed while standing comfortable (EC-CS); eyes open while standing in a narrow stance with feet together (EO-NS); eyes closed while standing in a narrow stance with feet together (EC-NS). For all trials, subjects wore a safety harness attached to a safety structure. Center of pressure (COP) data was collected for both the anterior-posterior direction and the medial-lateral directions. All trials were collected for sixty seconds at 1000 Hz, with data recorded on a laptop connected to the platform by a USB cable. On the occasion that balance was lost during a trial, the trial was marked as a failed attempt and that trial data was not used for further analysis. Figure 1 shows the testing set-up.

![Figure 1. Testing Set-up](image)

*Data Analysis and DFA Methodology*

To determine the fractal properties of the data collected, the directional sway component data for each trial was analyzed using Detrended Fluctuation Analysis to compute the fractal dimension. The original Detrended Fluctuation Analysis code, developed by C.K. Peng, and available through the NIH-sponsored website PhysioNet (www.physionet.org) was used for analysis [21,22].

For a comprehensive background of DFA, reference [22] is recommended. In summary, Detrended Fluctuation Analysis is a multi-step process, with the first step being to cumulatively sum the raw data series according to equation (1), where $B(i)$ is the data point of interest, $B_{ave}$ is the average value of the data, and $k$ ranges from 1 to N, the total number of data points:

$$y(k) = \sum_{i=1}^{k} [B(i) - B_{ave}]$$  

(1)
The cumulatively summed data is then broken up into equally sized windows, known as boxes, the size of which is \( n \). A best fit line is fit to the data contained in each window, and the data is detrended by subtracting this trend from the data in the box. The root mean square fluctuations of the data, \( F(n) \), are then found according to equation (2), where \( y_n(k) \) corresponds to the best-fit line.

\[
F(n) = \sqrt{\frac{1}{N} \sum_{k=1}^{N} [y(k) - y_n(k)]^2}
\]  

(2)

This process is repeated for various box sizes, \( n \), to determine the associated root-mean-square fluctuations, \( F(n) \). These values are then plotted on a log-log scale, and for signals with fractal qualities a linear region emerges. The slope of this region is known as the \( \alpha \)-scaling exponent and the value of this exponent characterizes the postural sway pattern. An \( \alpha \)-scaling exponent is typically a value between 1 and 2, with values of 1 being associated with strong anti-persistent trends and values of 2 being associated with strong persistent trends. A value of 1.5 indicates a random trend. The Detrended Fluctuation Analysis results for an arbitrary signal generated to demonstrate fractal properties are shown in Figure 2.

![Figure 2. Characteristic Detrended Fluctuation Analysis Plot for Arbitrary Fractal-Generated Signal](image-url)

Detrended Fluctuation Analysis was performed separately on the anterior-posterior and medial-lateral center of pressure data for all trials. From the Detrended Fluctuation Analysis, the \( \alpha \)-scaling exponent was to be recorded; however, the unexpected findings of two scaling regions, as discussed in the Results section, required modification to this analysis. Paired t-tests were performed for all resulting fractal characteristics for each sway direction and each testing condition to determine between-group differences (\( p < 0.05 \)).

**RESULTS**

*Presence of Two Scaling Regions*

Detrended Fluctuation Analysis plots for both repeat fallers and non-repeat fallers for all testing conditions and both sway directions revealed a novel and unexpected presence of two linear regions. Figure 3 shows a representative plot exhibiting the notable deviation from linear, suggesting two unique scaling regions.

![Figure 3. Representative Detrended Fluctuation Analysis Results Showing Two Linear Regions](image-url)

*Subsequent Analysis of Two-Scaling Regions*

To properly characterize the data, the linear regions were separately defined. The left-most linear region shown in Figure 3 was associated with box sizes that were very small, containing short time intervals of data. This became known as the short-term scaling region. The right-most linear region of Figure 3 was associated with box sizes that were much larger, containing longer time intervals of data. This became known as the long-term scaling region.

To determine the respective \( \alpha \)-scaling exponents, a Matlab code was used that optimized the intersection of the two scaling regions. The code iteratively broke the data into two distinct sets. Each set was fit with best fit lines and the coefficient of determination, \( R^2 \), was calculated to determine fit. This process was repeated for all possible points to find the crossover point where \( R^2 \) was maximized. Once this point was identified, the regions were then defined and the slope of each was found. To characterize the data the short-term \( \alpha \)-scaling exponent, the
long-term $\alpha$-scaling exponent, and the crossover point were then recorded. Figure 4 shows a representative plot with the two scaling regions optimized. Statistical analysis was then conducted as planned.

![Graph showing Detrended Fluctuation Analysis Results](Image)

**Figure 4.** Representative Detrended Fluctuation Analysis Results to Obtain Scaling Exponents. Dashed Line is Short-Term Scaling Region, Solid Line is Long-Term Scaling Region, Intersection is the Crossover Point

### Between-Subject Group Results

Table 1 gives the mean $\alpha$-scaling exponents and crossover points for the group who had experienced multiple falls and the group who had not for the anterior-posterior direction. Statistical analysis revealed that there were statistically significant between-group differences ($p < 0.05$) for the anterior-posterior short-term $\alpha$-scaling exponent for the eyes closed, comfortable stance condition and for the anterior-posterior crossover point for the eyes closed, narrow stance condition. No other fractal measures were found statistically different between the two groups.

### Effect of Sampling Frequency and Trial Duration

To determine why the findings of this study revealed two unique scaling regions and other studies did not, the effect of sampling frequency and trial duration were examined. This study collected data at a higher frequency (1000 Hz.) and longer trial duration (60 seconds) than previously published studies of Detrended Fluctuation Analysis of postural sway data [4,20]. As fractal analysis depends on the underlying trends in data the collection of more data samples, by increasing frequency and length of data collection is advantageous in getting a more accurate view of the data.

### Table 1. Mean Values for the Anterior-Posterior Short-Term $\alpha$-Scaling Exponent (ST $\alpha$), Long-Term $\alpha$-Scaling Exponent (LT $\alpha$), and Crossover Point (CP) for all Conditions

<table>
<thead>
<tr>
<th></th>
<th>Repeat Fallers</th>
<th>Non-Repeat Fallers</th>
<th>p-value</th>
</tr>
</thead>
<tbody>
<tr>
<td>ST $\alpha$</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>EO-CS</td>
<td>1.83 ± 0.04</td>
<td>1.82 ± 0.06</td>
<td>0.211</td>
</tr>
<tr>
<td>EC-CS</td>
<td>1.85 ± 0.04</td>
<td>1.82 ± 0.06*</td>
<td>0.010*</td>
</tr>
<tr>
<td>EO-NS</td>
<td>1.83 ± 0.05</td>
<td>1.82 ± 0.05</td>
<td>0.532</td>
</tr>
<tr>
<td>EC-NS</td>
<td>1.83 ± 0.06</td>
<td>1.82 ± 0.05</td>
<td>0.557</td>
</tr>
<tr>
<td>LT $\alpha$</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>EO-CS</td>
<td>0.93 ± 0.18</td>
<td>0.99 ± 0.24</td>
<td>0.262</td>
</tr>
<tr>
<td>EC-CS</td>
<td>0.88 ± 0.21</td>
<td>0.94 ± 0.21</td>
<td>0.381</td>
</tr>
<tr>
<td>EO-NS</td>
<td>0.90 ± 0.19</td>
<td>0.98 ± 0.20</td>
<td>0.114</td>
</tr>
<tr>
<td>EC-NS</td>
<td>0.89 ± 0.15</td>
<td>0.86 ± 0.19</td>
<td>0.554</td>
</tr>
<tr>
<td>CP</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>EO-CS</td>
<td>2.94 ± 0.23</td>
<td>3.02 ± 0.28</td>
<td>0.207</td>
</tr>
<tr>
<td>EC-CS</td>
<td>2.88 ± 0.21</td>
<td>2.95 ± 0.21</td>
<td>0.237</td>
</tr>
<tr>
<td>EO-NS</td>
<td>2.89 ± 0.17</td>
<td>2.94 ± 0.22</td>
<td>0.384</td>
</tr>
<tr>
<td>EC-NS</td>
<td>2.86 ± 0.10</td>
<td>2.95 ± 0.20*</td>
<td>0.033*</td>
</tr>
</tbody>
</table>

To determine the effect of trial duration, a representative trial was analyzed for both the first 10 seconds and the first 30 seconds, common values used in the analysis of center of pressure data. This was then compared to the original 60 second analysis. A single best fit line was fit to each resulting Detrended Fluctuation Analysis plot. Figure 5 shows this comparison. With increasing trial duration, the deviation from linear becomes increasingly distinct. The norm of the residuals further supports this, being 0.893 for 10 seconds, 1.873 for 30 seconds, and 2.461 for 60 seconds.

Downsampling the original 60 seconds of data to 100 Hz changed the value of the scaling exponents obtained by DFA, but did not change the presence of the two scaling regions. Thus, it appeared the scaling regions were tied to trial duration and not sampling frequency.

### DISCUSSION

One of the most important findings of this study is the presence of two scaling regions in Detrended Fluctuation Analysis plots of center of pressure. This finding allows better characterization of postural sway, while indicating potential modes of postural control. The $\alpha$-scaling exponents revealed that for very short time intervals, of less than a second as associated with crossover points of approximately 2.9, individuals exhibit a persistent pattern of sway. For balance this indicates that an individual whose center of pressure displaces will continue this displacement, rather than attempting to recover back to an equilibrium position. It appears that this pattern is not reliant on feedback, operating under a seemingly open-loop control. For longer periods of time, greater than a few seconds, individuals then switch to exhibiting an anti-persistent sway pattern. For balance this indicates that an individual experiences continuous oscillation in an attempt to...
keep an equilibrium position, and that movements away from equilibrium are countered with movements back. This indicates that in this longer-term scenario, individuals are relying on feedback, operating under a seemingly closed-loop control. It should be noted that the values obtained, particularly for the repeat-faller group, are outside of the typical range for $\alpha$-scaling exponents. It is expected that increasing the trial duration to 90 seconds would allow better line-fitting and characterization, reducing the high variability observed for this variable.

The findings of this study are novel for Detrended Fluctuation Analysis, but are supported by the work of others. For example, Peng et al. has found two scaling regions present in Detrended Fluctuation Analysis plots of heartbeat, revealing novel information about the underlying cardiac function [22]. Duarte and Zatsiorsky have found Detrended Fluctuation Analysis plots of unconstrained long-duration (15 minute) standing to also demonstrate two scaling regions [23]. Most notably however, is the relationship between the findings of this study and the work of Collins and De Luca using Stabilogram Diffusion Analysis [20]. Despite the long standing contention of the SDA method, the similarities between the findings of the two methods indicate that the postural sway characteristics suggested by Collins and De Luca, and supported by the current findings, indeed appear accurate. This serves to initiate further discussion between the two methods and may bring about better agreement and understanding about the nature of underlying postural control.

The use of fractal analysis to examine the underlying characteristics of sway was useful in this study in that differences in postural sway patterns between older adults who had suffered repeated falls and those who had not were identified. These statistically significant differences occurred in the anterior-posterior direction, with eyes closed. This provides interesting insight into the possible causes of postural instability that contribute to falls. It appears that individuals at high-risk of falling have a strong visual reliance, such that differences between the two groups are not noted when eyes are open but become apparent when vision is not available. As balance is dependent on appropriate visual, vestibular, and proprioceptive feedback, it is likely that impairment in the latter two contribute to the significantly greater persistent sway pattern that is observed in repeat fallers with eyes closed. This supports work by Maki et al. and Melzer et al. who have suggested that a loss of cutaneous sensation in the feet, leading to poor proprioception, is responsible for many falls in older adults [24,25].

Previous Detrended Fluctuation Analysis results of center of pressure by Norris et al. have also demonstrated differences between older individuals at high-risk of falling and those with low-risk of falling [4]. This study, however, collected data for only 30 seconds. The resulting data was treated as a single linear region, and a single $\alpha$-scaling exponent was reported. These findings led the authors to conclude that older adults

Figure 5. Effect of Trial Duration; Best-Fit Lines for 10 sec (top), 30 sec (middle), and 60 sec (bottom)
exhibited anti-persistent sway patterns, with the high-risk group exhibiting the most extreme of this type of pattern. In light of the current findings, it appears that the analysis by Norris et al. did not capture the underlying complexity of postural sway. The nature of sway reported by Norris captured only an anti-persistent pattern, rather than the two distinct patterns identified in the current study. This is in part due to the trial duration used. Though not acknowledged by the authors, the figure in Norris and colleague’s published work, shows a noticeable deviation from linear at 30 seconds, particularly for the high-risk group. This looks similar to the results obtained in the current study for 30 seconds, shown in Figure 5 [4]. Also notable, a review of the Detrended Fluctuation Analysis code used by Norris, indicated that the best-fit line was weighted toward the larger window sizes because the number of data points were not equally distributed along the log scale [26]. This indicates that the anti-persistent trend identified, is likely more representative of the start of this linear deviation, or as described in the current paper, the long-term scaling region. This suggests that results of Norris et al. are not as contradictory to the current findings as they may seem, while also suggesting the need for a thorough analysis to capture the true underlying patterns of sway.

The results of this study indicate the need to be cautious with the selection of data collection parameters, especially when newer methods such as fractal analysis are being used. Collecting data for too short of a duration may limit the information obtained, such that underlying patterns at different time scales go unrecognized. As fractal analysis grows in use as a powerful tool in fields as diverse as finance, hydrology, and medicine, and specific to engineering in a wide range of signal processing applications, it is especially important to carefully consider the signal to be monitored and how it would best be captured. This will ensure that the true potential of fractals, the ability to capture the underlying trends in data, are recognized. This also highlights a limitation of fractal analysis in diverse applications. Unless a standard data collection protocol is established, findings are not readily comparable to other similar findings. This is especially problematic for clinical applications, where long-term monitoring of fractal dimensions to signify declines in health would be ideal. The findings of this study show that apparent differences in fractal dimension from one measurement to the next could actually be due to changes in sampling frequency and trial duration, rather than intrinsic breakdown of postural sway patterns. It is, therefore, important that ensuring consistency by standardizing data collection is a focus of researchers using fractal methods.

Future work is necessary to address these concerns. In particular, it is necessary to perform a detailed study to determine what trial duration is optimum to capture postural sway data for fractal analysis. Care must be taken when determining this as to ensure capture of significant data while avoiding effects of fatigue associated with long duration stance. Future work will also seek to determine whether significant differences due to differences in sampling frequency are present in the data.

This paper has shown that fractal analysis of postural sway has the ability to distinguish individuals based on fall history, while also revealing information about the likely control of postural sway. It has also shown that care must be taken in determining trial duration and sampling frequency for consistent results. These findings translate outside of the specific field of balance and mobility, however. Fractals have been applied to a number of engineering problems ranging from turbulent flow analysis to the monitoring of oil production [27,28]. It is the hope of this paper that engineers from diverse fields consider whether fractal analysis has similar potential to provide additional insight into the work they are doing, especially work related to time-series data and signal processing. If so, the same care should be taken in considering the data acquisition parameters as identified for the specific case of center of pressure data, to ensure the most meaningful results.

CONCLUSIONS

Detrended Fluctuation Analysis results of postural sway data indicated that postural control is more complex than previously contended. Two unique patterns were identified, suggesting that individuals may use an open-loop control for short time periods and switch to a closed-loop control for longer time periods.

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REFERENCES


DESIGN & MANUFACTURING WITH MODELING, DYNAMIC BALANCING & FINITE ELEMENT ANALYSIS OF ROTARY FIXTURE FOR CNC TURNING CENTRE TO FUNCTION AS HMC

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ABSTRACT
Jigs and fixtures are the special production tools which make the standard machine tool, more versatile to work as specialized machine tools. They are normally used in large scale production by semi-skilled operators; however they are also used in small scale production when interchangeability is important.

Manufacturing industries have brought lot of revolutions in manufacturing technology, as a consequence of which several developments like CNC lathes, CNC machine centre, flexible manufacturing systems, fabrication centre, transfer machines, robotics etc. took place. Even with these advancements in the manufacturing industries, there is a continued use of jigs and fixtures in some form or the other either independently or in combination with other systems.

Various areas related to design of fixture are already been very well described by various renowned authors, but there is a need to couple and apply all these research works to an industrial application. This paper integrates all these aspects and the evolutionary functional approach of designed fixture is proved from the fact that a real industrial component is considered for fixture designing.

The component is Flow TEE body of petroleum refinery. The operations to be performed are front facing, outside diameter turning, grooving, boring and back facing. The research work of this paper is proved from the fact that 10 million rupees are saved in installation cost as now these operations can be performed on CNC turning centre instead of HMC using the designed fixture.

The paper presents the integrated approach of design for manufacturing. The research work includes the 3D assembled & exploded view of fixture using Pro/Engineer Wildfire 4.0. Fixture is mass balanced using Pro/Mechanism. Finite element analysis of fixture using Pro/Mechanica is also covered. The present volume of the paper also couples the research work and manufacturing. The real time application of the research reflects from the fact that a fixture is not only designed but mass balanced and manufactured also.

Key-words: Dynamic balancing, finite element analysis, rotary fixture, CNC (Computerized numerical control) turning centre, HMC (Horizontal machining centre)

INTRODUCTION
The machine tool industry has undergone sufficient changes as the requirement of user engineering systems changed; first it started with the manufacture of basic general purpose machine tools. These machines though offered higher flexibility were not suitable for mass production owing to longer set up times and the tedious adjustments of machine and tools besides requiring highly skilled operators.

With growing need of fast production to meet the requirement of industry, mass production machines are conceived. Hydraulic, tracer control machine tool, special purpose automatic and semi automatic machines were introduced with the advancement of technology. These machines were highly specialized but inflexible. The use of these machines was with a success for mass production and they have considerably reduced the production costs by way of reduced machining times and labor costs. Because of inflexibility these machine tools could not however be adopted by units involved in small lot and piece production.

Because of the above, great need is felt for tools that could bridge the gap between highly flexible general purpose machine tools (which are not economical for mass production) and highly specialized, but inflexible mass production machines. Numerical control machine tools with proper fixture set up have to take up this role very well. And this has excited this research work on application of fixture to change CNC turning centre to perform operations like on HMC. The present volume of
this paper includes the unique aspect of design, modeling & mass balancing of rotary fixture for CNC turning centre to function as HMC. CNC turning centre with designed fixture set up is economical for producing single or a large number of jobs. The use of designed fixture has avoided the installation cost of HMC as now all operations can be well performed on existing CNC turning centre.

The fixture designing and manufacturing is considered as a complex process that demands the knowledge of different areas, such as geometry, tolerances, dimensions, procedures and manufacturing processes. While designing this work, a good number of literature and titles written on the subject by renowned authors are referred. All findings and conclusions obtained from the literature review and the interaction with fixture designers are used as guide to design the present research work.

As stated by Koji Teramoto et al. [1], Fixturing Plan (FP) and Machining Plan (MP) are mutually dependent. Implicit to this conclusion, paper coordinates MP and FP by coupling a fixture designing with manufacturing, mass balancing and finite element analysis. For this research, a relevant issue when considering requirements, taking this as a general concept, is to make explicit the meaning of two main terms: Functional Requirement (FR) and Constraint (C) [2]. Functional Requirement (FR), as it stated by different authors, “represents what the product has to or must do independently of any possible solution”. Constraint (C) can be defined as ‘a restriction that in general affects some kind of requirement, and it limits the range of possible solutions while satisfying the requirements’. Adapting to this functional approach, the functional requirements is mass balanced rotary nature of fixture. Constraint is the use of only CNC turning centre, with component rotating and tool stationary.

Various areas related to design of fixture like machining fixture knowledge, optimizing workpiece setups, modeling of forces, improving workpiece location and high efficiency tools [3-7] are already been very well described by various renowned authors, this paper integrates all these research works and transforms the theoretical knowledge of fixture design to practical application by designing a fixture for a real industrial component - Flow TEE body of petroleum refinery.

The balancing of mechanisms is motivated by continuous interest machine designers express in the solution of problems concerning prevention of noise, wear and fatigue generated by the transmission of unbalanced shaking forces and shaking moments to the frames and foundations of machines. It generally confines itself to the shaking force and shaking moment balancing, full or partial, by internal mass redistribution or counterweight addition. However, the complete shaking force and shaking moment balancing problem is very complicated. Often in practice, the problem of mass balancing is limited by full force balancing and partial moment balancing [8]. In this work, fixture is balanced by adding counterweight equal in magnitude and opposite in direction as that of resultant unbalanced mass. The object of the work presented here is to develop the study and to provide the optimum conditions of design, manufacturing, static analysis with force & moment balancing of fixture.

STATEMENT OF PROBLEM

“Design & manufacturing of fixture for machining flow TEE body on CNC turning centre. The operations to be performed are front facing, outside diameter turning, grooving, boring and back facing. The fixture being rotary in nature has to be balanced.”

COMPONENT DETAILS

The methodology proposed for design of a fixture includes the realization of two stages. The first stage represents the knowledge of the objects like part geometry, machining process, functional and detailed fixture design, and fixture resources. The second stage describes the inference process (design and interpretation rules) needed to obtain a first solution for the machining fixture [3]. As a part of first stage, component geometry is discussed here [Figure 1-4]. The component is Flow TEE body, made up mild steel, weighing 46.5 kg and is one of the components of petroleum refinery. The component is used as a joint or coupler for pipes through which petroleum liquid products flows and mixes. The component in raw material form is forged, proof machined with 3 mm machining allowance on conventional lathe with 24 inch swing over diameter. The operations to be performed on component, using designed fixture set up, are front facing, outside diameter turning, grooving, boring and back facing on one circular face.
DESIGN OF FIXTURE – LOCATION AND CLAMPING CONSIDERATIONS

Workpiece location in a fixture is significantly influenced by localized elastic deformation of the workpiece at the fixturing points. These deformations are caused by the clamping force(s) applied to the workpiece. For a relatively rigid workpiece, the localized elastic deformations cause it to undergo rigid body translations and rotations which alter its location with respect to the cutting tool. It is therefore important to minimize such effects through optimal design of the fixture layout [6].

In machining, work holding is a key aspect, and fixtures are the elements responsible to satisfy this general goal. Usually, a fixture solution is made of one or several physical elements, as a whole the designed fixture solution must satisfy the entire FRs and the associated Cs. Centering, locating, orientating, clamping, and supporting, can be considered the functional requirements of fixtures. In terms of constraints, there are many factors to be considered, mainly dealing with: shape and dimensions of the part to be machined, tolerances, sequence of operations, machining strategies, cutting forces, number of set-ups, set-up times, volume of material to be removed, batch size, production rate, machine morphology, machine capacity, cost, etc. At the end, the solution can be characterized by its: simplicity, rigidity, accuracy, reliability, and economy.

Workpiece motion arising from localized elastic deformation at the workpiece/fixture contacts due to machining and clamping forces significantly affect the workpiece location accuracy and hence the machined part quality. Contact problems with friction are generally complicated by the fact that the contact surface can experience slipping, sliding, rolling or tension release depending on the magnitude of the normal and tangential forces at the contact interface [9].

Considering all above mentioned facts, the complete locating & clamping is accomplished by using 3 V blocks and latch clamp. The important parts of fixture used here are V block, latch clamp, base plate, vertical plate, adapter plate, locator and rib. The fixture uses three V blocks to locate the component and a latch clamp to hold the component. The latch clamp consists of two M 6 bolts to directly clamp the workpiece. The chuck of CNC turning centre will be replaced with complete fixture setup using an adapter plate. The adapter plate holds the same dimensions of chuck plate. The locator locates the vertical plate in correct position with adapter plate. The base plate serves to hold the complete assembly of fixture. The ribs are clamped to base plate and provide the holding arrangement for latch clamp. The complete fixture assembly of total weight 256.71 kg including component weight of 46.5 kg and balancing weight of 23.59 kg rotates with 550 rpm while performing...
operations on CNC turning centre. The specification of spindle nose of CNC turning centre used in this work is A2-8, which can carry a weight of 450 kg. The fixture is directly mounted on spindle nose.

Figure 5. 3D view of fixture assembly without component

Figure 6. 3D view of fixture assembly with component

Figure 7. 3D rear view of fixture assembly

Figure 8. 2D drawing of fixture assembly
BALANCING OF FIXTURE

As the fixture is asymmetrical, it has to be mass balanced. The fixture rotates around one axis; hence it has to be balanced about other two perpendicular axis. Here x – axis is the axis of rotation. The innovative approach of use of Pro/Engineer Wildfire 4.0 is used to solve the balancing problem. The results and outputs from Pro/Engineer Wildfire 4.0 with solution of balancing are shown below.

Step I: C. G., weight of fixture and offset distance of C. G. from axis of rotation are determined [Figure 10].

Figure 10. Mechanics analysis with component

The important results from the above output are as follows: Weight of fixture with component, without balancing mass = 233.12 kg. C. G. is offset from axis of rotation in x – axis by -130.56 mm, in y – axis by -1.11 mm and in z – axis by 2.38 mm.

Step II: Now the fixture is cut in 4 quadrants around 2 axis, perpendicular to each other and perpendicular to axis of rotation below [Figure 11].

Step III: The weight of the fixture and C. G. in each quadrant is determined. [Figure 12-15].

Step IV: The above outputs of weight of fixture and C. G. of each quadrant are summarized [Figure 16].

Figure 9. 3D exploded view of fixture assembly

Figure 11. 3D view of fixture in 4 quadrants

Figure 12. Weight of fixture and C. G. in Quadrant 1

Figure 13. Weight of fixture and C. G. in Quadrant 2

Figure 14. Weight of fixture and C. G. in Quadrant 3

Figure 15. Weight of fixture and C. G. in Quadrant 4
Figure 16. 2D drawing of summary of weight of fixture and C. G. in all quadrants

Step V: According to principles of mechanics, $\Sigma F = 0$ and $\Sigma M = 0$ for mass balancing. The sum of unbalanced mass in horizontal direction $\Sigma F_H$ and in vertical direction $\Sigma F_V$ is calculated to start with.

Table 1. Calculation of resultant mass in horizontal direction ($\Sigma F_H$) and in vertical direction ($\Sigma F_V$)

<table>
<thead>
<tr>
<th>Quadrant (i)</th>
<th>$m_i$ (kg)</th>
<th>$F_{H,i} = m_i \cos \theta_i$ (kg)</th>
<th>$F_{V,i} = m_i \sin \theta_i$ (kg)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>38.5</td>
<td>26.73222374</td>
<td>27.7053199</td>
</tr>
<tr>
<td>2</td>
<td>48.09</td>
<td>-38.1322274</td>
<td>30.035257</td>
</tr>
<tr>
<td>3</td>
<td>53.36</td>
<td>-42.6751489</td>
<td>-26.302374</td>
</tr>
<tr>
<td>4</td>
<td>43.82</td>
<td>31.2075185</td>
<td>-30.761716</td>
</tr>
<tr>
<td>$\Sigma$</td>
<td></td>
<td>$22.8682006$</td>
<td>$-5.7885129$</td>
</tr>
</tbody>
</table>

Step VI: Resultant unbalanced mass ($R$) and its line of action in terms of angle ($\alpha$) with x-axis are calculated using parallelogram law of forces.

Table 2. Calculation of Resultant force, $R$

<table>
<thead>
<tr>
<th>$\Sigma F_H^2$</th>
<th>522.9546 kg$^2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Sigma F_V^2$</td>
<td>33.5068 kg$^2$</td>
</tr>
<tr>
<td>$\Sigma F_H^2 + \Sigma F_V^2$</td>
<td>556.46146 kg$^2$</td>
</tr>
<tr>
<td>Resultant, $R$</td>
<td>$23.589435$ kg</td>
</tr>
<tr>
<td>$\tan \alpha$</td>
<td>0.253125</td>
</tr>
<tr>
<td>$\alpha$ (Radian)</td>
<td>0.2478539 radian</td>
</tr>
<tr>
<td>$\alpha$</td>
<td>14.200985$^\circ$</td>
</tr>
</tbody>
</table>

Step VII: Sum of moment of inertia about x – axis ($\Sigma m_i x_i^2$) and that about y – axis ($\Sigma m_i y_i^2$) are calculated.

Table 3. Calculation of sum of moment of inertial about x – direction ($\Sigma m_i x_i^2$) and that of about y– direction ($\Sigma m_i y_i^2$)

<table>
<thead>
<tr>
<th>Quadrant (i)</th>
<th>$m_i$ (kg)</th>
<th>$m_i x_i^2$ (kg mm$^2$)</th>
<th>$m_i y_i^2$ (kg mm$^2$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>38.5</td>
<td>265802.002</td>
<td>3543.54</td>
</tr>
<tr>
<td>2</td>
<td>48.09</td>
<td>510186.81</td>
<td>3884.7102</td>
</tr>
<tr>
<td>3</td>
<td>53.36</td>
<td>545835.427</td>
<td>4127.396</td>
</tr>
<tr>
<td>4</td>
<td>43.82</td>
<td>297166.316</td>
<td>3755.8122</td>
</tr>
<tr>
<td>$\Sigma$</td>
<td></td>
<td>1618990.55</td>
<td>15311.4584</td>
</tr>
</tbody>
</table>

Step VIII: Resultant moment is calculated using principle of perpendicular axis theorem of moment of inertia.

Table 4. Calculation of Resultant moment, $M$

| $I_{xx} = \Sigma m_i x_i^2$ | 1618990.55 kg mm$^2$ |
| $I_{yy} = \Sigma m_i y_i^2$ | 15311.45 kg mm$^2$ |
| $I_{zz} = I_{xx} + I_{yy}$ | 1634302.00 kg mm$^2$ |

| $M = \Sigma m_i x_i^2 + \Sigma m_i y_i^2$ | 1634302.00 kg mm$^2$ |

Step IX: Having $M$, $R$ and $\alpha$, the location of C. G. ($r_{cm}$) of $R$ is determined.

$$M = R r_{cm}^2$$

$\Rightarrow r_{cm}^2 = M / R$

$\Rightarrow r_{cm} = 69281.09$

$\Rightarrow r_{cm} = 263.21$ mm

Thus the unbalanced mass is found to be 23.59 kg and its C. G. is situated at an angle of 14.20$^\circ$ with x-axis at a distance of 263.21 mm in quadrant 3. Hence the fixture can be balanced by placing the counterweight equal in magnitude and opposite in direction as that of unbalanced mass.

**CALCULATION OF CUTTING FORCE**

As main operation to be performed on component is outside diameter turning and maximum cutting force acts for this operation; calculation [10] is made for the same. The data of cutting conditions are as under:

$D =$ Diameter of face of workpiece = 223.4 mm,
$n =$ revolutions per minute = 550,
$s =$ Feed per revolution = 0.3 mm / rev,
t = Depth of cut = 0.75 mm,
x = Approach angle = 45°,
U = Unit power = 0.03 kW/cm³/min,
g = gravitational acceleration = 9.8 m/s²

Cutting speed, \( v = \frac{\pi D n}{1000} \)
\[ \Rightarrow v = 386 \text{ m/min} \] (2)

Feed per minute, \( S_m = s n \)
\[ \Rightarrow S_m = 165 \text{ mm / min} \] (3)

Metal removal rate, \( Q = stv \)
\[ \Rightarrow Q = 86.85 \text{ cm³/min} \] (4)

Average chip thickness, \( a_s = s \sin x \)
\[ \Rightarrow a_s = 0.212 \text{ mm} \] (5)

For, component material of mild steel, HB = 300, \( a_s = 0.212 \text{ mm} \) and assuming flank wear of 0.2 mm, Correction factor for flank wear, \( K_h = 1.09 \). For Rake angle = 10°, Correction factor for rake angle \( K_\gamma = 1 \) [10].

Power at the spindle, \( N = U x k_h x k_\gamma x Q \)
\[ \Rightarrow N = 2.84 \text{ Kw} \] (6)

Assuming, Efficiency of transmission, \( E = 85 \% \)

Power of the motor, \( N_{el} = N / E \)
\[ \Rightarrow N_{el} = 3.34 \text{ Kw} \] (7)

Tangential cutting force, \( P_z = 6120N g / v \)
\[ \Rightarrow P_z = 519.49 \text{ N} \] (8)

Torque at the spindle, \( T_s = 975 x N / n \)
\[ \Rightarrow T_s = 58.07 \text{ N.m} \] (9)

As cutting force is only 519.49 N, two M6 bolts with clamping force of 2.5 kN each is used to clamp the workpiece.

**STRESS ANALYSIS**

Stress analysis is carried out on major components of fixture like adapter plate, rib and V block using Pro/Mechanica. In the analysis shown below, resultant force due to weight of fixture, centrifugal force and cutting force is considered along with moments due to weight of fixture and centrifugal force.

**CONCLUSION**

An integrated approach of manufacturing, mass balancing and stress analysis to the design process of rotary fixture has been adopted in this work. This approach is of crucial importance in real manufacturing environment. Actually HMC is the best solution for performing the required operations on part used in this work, but a designer cannot ask industry to replace already existing set up of CNC turning centre with HMC. Moreover, HMC costs around 12.5 million rupees.
whereas CNC turning centre costs only about 2.5 million rupees. Here the research work of this paper is proved, 10 million rupees are straight away saved in machine installation cost as these operations now can be performed on CNC turning centre using the designed fixture. In HMC, a tool rotates and component remains stationary, vice versa for CNC turning centre. A designed fixture has the important novel characteristic of performing all operations in a single set up with component rotating and tool stationary, satisfying the essential requirement of CNC turning centre.

A simplified, analytical method of use of Pro/Engineer Wildfire 4.0 is proposed to solve the balancing problem. The approach of application of Pro/Engineer Wildfire 4.0 to mass balance the fixture is very useful as it opens the door not only to symmetrical part problems but also to difficult tasks such as asymmetrical fixture as is the case in this paper. The application of Pro/Engineer Wildfire 4.0 and principles of mechanics used in this work to overcome balancing problem is universal i.e applicable for any part. The findings of unbalanced mass and its location of C. G. is remarkably same as with experimental results. This approach of solving the balancing problem is expected to have more flexibility in its application, since it is not sensitive to dynamic conditions. However, the analytical results are very encouraging. Stress analysis shows that maximum stress of 57.66 N/m² acts on adapter plate which is much less than shear strength of five bolts used to hold the adapter plate, proving the fixture safe in operation.

FUTURE SCOPE
Second set up of fixture can be designed for performing same operations on another circular face of the component. The face machined using the present fixture set up can be used for locating the component.

ACKNOWLEDGEMENT
The authors wish to acknowledge the support of Mr. Sudhir Thakar and Mr. Pradip Thanki, Trend incorporation, Rajkot, Gujarat, India for this research work.

REFERENCES
ABSTRACT
The paper details the optimization options, their combination under a set of defined constraints and a comparison between the original forged steel crankshaft and the final optimized forged steel component. The main objective of this analysis was to optimize the weight and manufacturing cost of the forged steel crankshaft, which not only reduces the final production cost of the component, but also results in a lighter weight crankshaft which will increase the fuel efficiency of the engine. Optimization carried out on this component is not the typical mathematical sense of optimization, because variables such as manufacturing and material parameters could not be organized in a mathematical function according to the set of constraints such that the maximum or minimum could be obtained. In this case of optimization process, the final optimized geometry has definitely less weight than the original crankshaft but this does not mean that the weight could not be reduced further. In other words, this may not be the minimum possible weight under the set of constraints defined. As the main objective of this analysis, it was attempted to reduce the weight and final cost of the component by changing the crankpin geometry, Increasing the oil hole diameter and fillet radius, Increasing the oil hole depth and Changing the crank web geometry.

The method describes the first step in the optimization process to reduce weight of the component considering dynamic loading, which means that the stress range under dynamic loading should not exceed the stress range magnitude in the original crankshaft. The optimization process was categorized in different stages and paper concludes with the sufficient reduction in weight and ultimately cost.

INTRODUCTION
The crankshaft is one of the most important components in the internal combustion (IC) engine and has a complex geometry consisting of cylinders as bearings, and plates as the crank webs. Geometrical changes in the crankshaft causes stress concentration at fillet areas where bearings are connected to the crank webs. In addition, this component undergoes both torsional and bending loads during its service life. Therefore, fillet areas are locations that are subject to the most critical stresses during the service life of the crankshaft. As a result, these locations are a common fatigue failure site of crankshafts. Since the crankshaft has a multifaceted geometry for analysis, finite element models have been well thought-out to provide an accurate and reasonable simulation. Because crankshafts are among large volume production components in the IC engine, weight and cost reductions of this component are very effective in improving the fuel efficiency and dropping the overall cost of the engine.

Since fatigue crack initiation and fracture at the fillets is one of the primary failure mechanisms of automotive crankshafts, the fillet rolling process has been used to improve the fatigue life of crankshafts for many years. The fillet rolling process induces compressive residual stresses within the fillet surface. The compressive residual stress lowers the fatigue driving forces due to operating loads near the fillet surface and consequently increases the fatigue life of the crankshaft.

A study was performed on the effect of fillet rolling on fatigue strength of a ductile cast iron crankshaft[1]. Bench tests were conducted on crankshaft pin samples with a fatigue evaluation on test pieces in order to study the fatigue strength of fillet rolled crankshafts and specimens. This study showed that an optimum deep rolling method could increase the bending fatigue strength by 83% over conventional ductile iron crankshafts that were not fillet rolled. Without any dimensional modification, the fatigue life of a crankshaft could be improved significantly by applying various surface treatments[2].

The specimens prepared from the crankshaft in the study found the optimum level of rolling force was experimentally to be between 7000N and 9000N. An extensive study was performed by Nallicheri et al. on material alternatives for the automotive crankshaft based on manufacturing economics [4]. Steel forgings, nodular cast iron, micro-alloy steel forgings, and austempered ductile iron (ADI) casting were considered as manufacturing options to evaluate the cost effectiveness of using these alternatives for crankshafts. It was concluded that the production volume of the crankshaft and the requirements of the engine were predominant factors in a cost effective production option for this application.

A study was performed by Hoffmann and Turonek[4] to examine the cost reduction opportunities associated with forged steel, materials evaluated in their study included
medium carbon steel SAE 1050 (CS) and medium carbon alloy steel SAE 4140 (AS) grades using a sulfur level of 0.10%, (CS-HS and AS-HS), and two micro-alloy grades (MA1 and MA2)[4]. The material selection was based on fatigue strength requirements and potential cost benefits. The micro alloy grades that were evaluated offered cost reduction opportunities over the original materials. The micro-alloy grade could reduce the finished cost by 11% to 19% compared to a quenched and tempered alloy steel (SAE 4140), and by 7% to 11% compared to a quenched and tempered carbon steel (SAE 1050). In addition, the micro-alloy grades met or exceeded the fatigue strength of the original materials for the applications studied and had better machinability characteristics.

Finite element analysis was used to obtain the variation in stress magnitude at critical locations. The dynamics of the mechanism was solved using analytical techniques and the results were verified by simulation in ADAMS, which resulted in the load spectrum applied to the crank pin bearing. The load was applied to the FE model in Pro Mechanica, and the boundary conditions were defined according to the engine mount design. The optimization carried out in this work was not based on only the typical geometrical optimization techniques. This is because variables such as manufacturing and material parameters could not be organized in a mathematical function according to the set of constraints such that the maximum or minimum could be defined.

Instead, each optimization step was approximated based on improving fatigue resistance while considering manufacturing feasibility and maintaining dynamic balance with an aim of reducing the weight and the final cost of the component.

**COMPONENT SPECIFICATIONS AND MANUFACTURING PROCESS**

In order to carry out optimization process, it is necessary to have knowledge of the component dimensions, its service conditions, and material of construction, manufacturing process, and other parameters that affect its cost. It was shown that the maximum bending load occurs at the lowest operating engine speed. Therefore, this loading condition was considered as the primary loading condition for the optimization study. The forged steel crankshaft material, AISI 1040, has the chemical composition shown in Table 1. As can be seen in this table, this high-strength low-alloy steel contains 0.45% carbon resulting in yield strength of 625 MPa and fatigue strength of 359 MPa at $10^6$ cycles.[5]

The main manufacturing process of the forged crankshaft is hot forging and machining. Each step of this processes is described below, where the information about the forging and machining processes were obtained from the metal forming books and OEM websites.

<table>
<thead>
<tr>
<th>Element</th>
<th>Percent by weight</th>
</tr>
</thead>
<tbody>
<tr>
<td>C</td>
<td>0.45</td>
</tr>
<tr>
<td>Mn</td>
<td>0.81</td>
</tr>
<tr>
<td>P</td>
<td>0.06</td>
</tr>
<tr>
<td>S</td>
<td>0.06</td>
</tr>
<tr>
<td>Si</td>
<td>0.27</td>
</tr>
<tr>
<td>Al</td>
<td>0.033</td>
</tr>
<tr>
<td>Cr</td>
<td>0.1</td>
</tr>
<tr>
<td>Ni</td>
<td>0.05</td>
</tr>
<tr>
<td>Cu</td>
<td>0.13</td>
</tr>
<tr>
<td>N</td>
<td>0.008</td>
</tr>
<tr>
<td>O</td>
<td>13 ppm</td>
</tr>
<tr>
<td>Fe</td>
<td>balance</td>
</tr>
</tbody>
</table>

1. The raw material samples of the AISI 1040 are inspected for chemical composition.
2. The material is shaped and cut to the rough dimensions of the crankshaft.
3. The shaped material is heated in the furnace to the temperature of 900°C to 1100°C.
4. The forging process starts with the pre-forming dies, where the material is pressed between two forging dies to get a rough shape of the crankshaft.
5. The forging process continues with the forging of the pre-formed crankshaft to its first definite forged shape.
6. Trimming process cuts the flash which is produced and appears as flat unformed metal around the edge of the component.
7. The exact shape of the forged crankshaft is obtained in the coining process where the final blows of the hammer force the stock to completely fill every part of the finishing impression.
8. The final shaped forged crankshaft is now ready for the shot cleaning process. In this step the scales remained from forging process are removed.
9. The machining process starts with the facing and centering of the total length size.
10. After alignment of all diameters the turning process will give a rough shape of cylinder to all cylindrical portions.
11. CAM turning is the process used to produce cylindrical components, typically on a lathe. A cylindrical piece of stock is rotated and a cutting tool is traversed along 2 axes of motion to produce precise diameters and depths. Turning can be either on the outside of the cylinder or on the inside (also known as boring) to produce tubular components to various geometries.
12. In the drilling operation, all inner diameters are drilled in the crankshaft geometry. The drilling mainly consists of oil holes.
13. Threads are cut on the inner surface of the bore at the back of the crankshaft and on the outer diameter of the front shaft.
14. Heat treatment is the next step to obtain the desired mechanical properties for the material.
15. Shot blasting consists of attacking the surface of a material with one of many types of shots. Normally this is done to remove scale from the surface.
16. Straightening process by application of external forces eliminates or reduces the curvatures, which can result by deformation during rolling, drawing, extrusion or due to non-uniform cooling. Thickness and geometry changes at different sections of a crankshaft cause non-uniform cooling during the forging process, which results in unwanted curvatures along the forged component.
17. After the straightening process the crankshaft is ready for grinding and being aligned to its final dimensions. Therefore, the grinding begins with the rough grinding of all diameters.
18. Since the crankshaft has eccentric cylinders the diameters have to be grinded using CAM.
19. The final grinding of diameters sets the cylinder diameters to their final acceptable tolerance. This is followed by grinding of other sections such as grooves using CAM.
20. The final step in grinding is face grinding, where the dimensions of the crankshaft will be finalized.
21. The last step in the machining process is balancing the crankshaft. In this process the crankshaft is mounted on two bearings in a device, and the dynamic balance of the component is checked. Mass and location of material removal is specified. Drilling holes in the counter weights will balance the crankshaft dynamically. The balance of the crankshaft is checked once more on the device.
22. Final washing of the component and preparation for final inspection.
23. The final inspection consists of checking diameter of cylinders, radius of crankshaft and distance of faces.
24. The finished forged crankshafts are sent for packing and dispatch.

As a main objective of the optimization study, the cost break down for each manufacturing step is very important. The influence of different parameters on the final cost of the component is another way for the cost break down. These parameters are shown in Table 2. Summarizing the manufacturing process to 12 steps are also listed in Table 2 helps in cost estimation of the manufacturing process. In this table, each manufacturing step and its share in the total cost is shown.

**DYNAMIC LOAD AND STRESS ANALYSIS**

The crankshaft is subjected to complex loading due to the motion of the connecting rod, which transforms two sources of loading, namely combustion and inertia, to the crankshaft. Optimization of the crankshaft requires a determination of an accurate assessment of the loading, which consists of bending and torsion. Dynamic loading analysis of the crankshaft results in more realistic stresses whereas static analysis provides results that may not reflect operating conditions. Accurate assessment of stresses is critical to the input of fatigue analysis and optimization of the crankshaft design.

Figure 1 shows the digitized model of the forged steel crankshaft created in Pro Engineer used for this study. The dynamic analysis of the engine that uses this type of crankshaft showed that as the engine speed increases the maximum bending load decreases. Therefore, the critical loading case for this engine is at the minimum operating speed of 2000 rpm [5]. This should not be misunderstood as to mean that the higher the engine rpm is the longer the service life because there are many other factors to consider in operation of the engine. The most important issue when the engine speed increases is wear and lubrication. As these issues were not considered in the dynamic load analysis study, further discussion of these issues is avoided.

![Figure 1 The Crankshaft modeled in Pro Engineer to be Optimized](image)
applying a unit load to each basic condition and then scaling the stresses from each unit load according to the dynamic loading. Then the corresponding stress components are added together. Figure 2 shows the maximum von Mises stress and von Mises stress range at six locations on the crankshaft fillets at the engine speed of 2000 rpm for the crankshaft. The sign of von Mises stress was determined by the sign of the principal stress that has the maximum absolute value. As can be seen from the figure, the maximum von Mises stress occurs at location 2, while other locations experience stresses lower than location 2. Therefore, the other five locations were not considered to be critical in the analysis.

OPTIMIZATION PROBLEM DEFINITION
At the beginning of this chapter it was mentioned that the optimization study performed on this component was not the typical mathematical optimization process. There are different functions and limitations in the mathematical optimization, which are all defined as a set of variables. The main objective function is minimizing the weight, maximum stress at critical locations, and manufacturing cost. Geometrical properties parameters such as thickness, diameter, and area are used as design variables in size optimization. There are other optimization methods such as Shape Optimization and Topological Optimization, which change the appearance of the geometrical domain. The optimization approach in this study involved both size and shape optimizations. As discussed earlier, the optimization stages were considered not as a defined function of variables, but based on judgment using the results of the FEA and dynamic service load.

OBJECTIVE FUNCTION
Objective function is defined as the parameters that are attempted to be optimized. In this study the weight, manufacturing cost and fatigue performance of the component were the main objectives. Optimization attempt was to reduce the weight and manufacturing cost, while improving the fatigue performance and maintaining the bending stiffness within permissible limits.

CONSTRAINTS
Since the current crankshaft used in the engine has proper fatigue performance, optimization was carried out in such a way that the equivalent local stress amplitude at any location of the optimized model did not exceed the equivalent stress amplitude at the critical location of the original model. Considering two stages for the optimization approach, the following constraints were defined for each stage.

Since the optimized crankshaft was expected to be interchangeable with the current one, the following dimensions were not changed:
- Outer diameters of different cylinders
- Crank radius
- Location of main bearings (distance between them)
- Geometry of main bearings
- Thickness and geometry of connecting rod bearing

DESIGN VARIABLES
Parameters that could be changed during the optimization process are design variables. Considering the functions of the crankshaft and its constraints, the following design variables were considered in the optimization study:

- Thickness of crank web
- Geometry of crank web
- Increasing inner hole diameters and depths
- Geometry changes on the outer part of crankpin bearing

Manufacturing process and material alternatives are other design variables that were considered in this study. This improvement would allow additional changes in the geometry in order to reduce the weight of the final optimized crankshaft.

GEOMETRY OPTIMIZATION PROCEDURE
The investigation of the stress contour of the crankshaft FEA model during an engine cycle showed that some locations of the crankshaft, such as the counter weights and crank webs, are subject to low stresses. The crankshaft has to be dynamically balanced in which the counter weights serve this purpose. Therefore, although stresses applied to these sections are low, these sections cannot be removed, but can only be changed according to other modifications made to the component.

Objective function, design variables, and constraints are summarized in this figure and it is shown that the optimization process consisting of geometry modifications, manufacturing process considerations, and material alternatives was performed simultaneously. Local shape optimization techniques were applied to different locations of the crankshaft to lower the weight. After each optimization step the counter weights were balanced in order to achieve an accurate estimate of the weight reduction. In a feasible design, the component stresses fall within the stress limits and bending stiffness does not change significantly, while the manufacturability is still economical.
According to FE analysis, the blue locations shown in Figure 3 have low stresses during the loading cycle and have the potential for material removal and weight reduction. It should be noted that the effect of mean stress on the results was negligible. Therefore, all of the stresses under consideration and discussed here are with reference to the stress ranges.

Figure 3: Stress distribution under critical loading condition

Several cases of geometric modifications were considered. Since maintaining dynamic balance is a key concern in the optimization of this component, the first step was to remove material symmetric to the central axis without compromising the dynamic balance of the crankshaft. On the far right side of the crankshaft shown in Figure 1 there is a threaded hole. The depth of this hole does not affect the function of the crankshaft. Therefore, this hole could be drilled as far as possible in the geometry (Case 1 in Figure 4). Another optimization step which does not require any complicated changes in the geometry is increasing the diameter of the crankpin hole (Case 2 in Figure 4). In order to balance the modified crankshaft, material has to be removed from the counter weight.

OPTIMIZATION USING GEOMETRY VARIABLES CONSIDERING DIFFERENT OPTIMIZATION CASES

Investigating the stress contour of the crankshaft FEA model during an engine cycle showed that some locations of the crankshaft experience lower stresses such as; counter weights and crank webs. Geometry optimization of the crankshaft results in weight reduction and therefore, reduction of the moment of inertia. In order to maintain the original dynamic behavior of the mechanism, the moment of inertia of the rotating components has to remain unchanged.

According to FE analysis, blue locations shown in Figure 3 have low stresses (85.9Mpa) during service life and have the potential for material removal and weight reduction. Therefore, the following optimization options were considered.

It should be added that the effect of mean stress in the results was negligible. Therefore, all stress concerns were about the stress range. The comparisons of before and after optimization is discussed in the three cases.

- **Case 1: Increasing the depth of the drilled hole at the back of the crankshaft**
  
  Since the dynamic balance is one of the main concerns in the optimization of this component as the first step it was tried to remove material symmetric to the central axis, which would not disturb the dynamic balance of the crankshaft. At the back of the crankshaft, there is a threaded hole. Therefore, this hole could be drilled as far as possible in the geometry. The current depth and the increased depth of this bore at the back of the crankshaft is shown in figure 4. As per the stress results for the critical location for different optimization cases, where value of mean stress is 73 MPa, stress range of 188MPa and 3.72 kg for weight. Therefore, each time a node is selected, a variation could be seen in the results.

- **Case 2: Increasing the hole diameter of the crankpin oil hole**
  
  Another optimization step which does not require any complicated changes in the geometry is increasing the hole diameter of the crankpin hole. Increasing the inner diameter of this hole will result in decreasing the moment inertia of the cross section. Therefore, in order to not increase the stress level at the fillet area, the fillet radius has to be increased. Considering this optimization option the stress range reduces by 5%, compared to the original model can be obtained. The reason for this reduction is increasing the fillet area, which causes a lower stress concentration factor. Weight reduction in this step is about 3%.

- **Case 3: Reducing the thickness of the web**
  
  A high weigh percentage of the crankshaft is in the crank web volume; therefore, reducing the weight of this section could result in a more efficient weight reduction of the component. Reducing the web thickness is another applied optimization case that was performed on the crankshaft web. As a result of this change in the crank web the center of gravity moves toward the crankpin bearing. This optimization case results in the maximum weight reduction of 7%. Since each optimization case was studied individually, further analysis was needed by considering a combination of these cases. Options for a redesigned crankshaft were developed such that as many optimization cases as possible could be applied.

Figure 4: Optimized crankshaft geometry with combination of case 1,2, and 3.
FE models of possible combinations were created and FE analysis with dynamic load was considered for each combination. The combination of Cases 1, 2, and 3 results in a 10% weight reduction in comparison with the original crankshaft.

Considering the manufacturing processes, the geometry of the crankshaft could be modified further to take advantage of the results of improved fatigue strength due to fillet rolling and/or the use of micro alloyed steel. These modifications reduce the weight of the original crankshaft by 18%. The final optimized geometry is shown in Figure 4.

It should be noted that the fatigue strength of the optimized crankshaft is significantly higher than the original crankshaft due to a slight increase in the stress range of 7% at the fillet and a significant increase on the order of 40% to 80% in fatigue strength due to fillet rolling, as discussed earlier. With regard to the cost of the optimized crankshaft, this is affected by the geometry changes and weight reduction, modification in the manufacturing process, and the use of MA steel. The optimized geometry requires redesign and remanufacturing of the forging dies used. Although a micro alloy steel grade is somewhat more expensive than hot-rolled steel bar, the heat treatment cost savings are significant enough to offset this difference.

In addition, micro alloyed steel has 5% to 10% better machinability than quenched and tempered steel, resulting in reduced machining costs due to enhanced production rates and longer tool life (Nallicheri et al. [4]). A consideration of these factors, along with the reduced material cost due to the 18% weight reduction, indicates a reduction in the total cost of the forged steel crankshaft.

MODIFICATION TO MANUFACTURING PROCESS

As the next step for the optimization study it is tried to modify the production steps in order to reduce the cost or improve the performance of the current crankshaft. Further improvement of the performance could result in more geometry changes and weight reduction. The optimization in this section was investigated by considering adding compressive residual stress to the fillet area of the crankpin.

Since the nitriding process is time consuming in comparison with other heat treatment processes, it was not considered as a modification to manufacturing process to increase the performance of the crankshaft. The fatigue bending moment for micro alloyed 35MV7 steel without surface treatment was 1990 N.m. As could be seen in this table, the fatigue strength increases by 87% and 125% by fillet rolling forces of 9 kN and 12 kN, respectively. For short nitriding treatments, the fatigue limit of micro alloyed 35MV7 steel increased by about 135%.

MODIFICATION USING ALTERNATIVES MATERIALS

One of the most common alternatives for the forged steel material is micro alloyed steel. A study was performed on a micro alloyed (MA) steel with titanium addition specially adapted for the production of forged crankshafts and which does not require any post-forging treatment[5]. Cost reduction of 13% is obtained for the final crankshaft by replacing the traditional AISI 4142 steel with 35MV7 control-cooled micro alloyed steel. This includes 10% savings on the unfinished piece, 15% saving on mechanical operations and 15% saving on ion nitriding treatment [5]. A comparison between the material properties used in the current crankshaft, AISI 1040 steel, and microalloyed steel 35MV7 indicates similar yield strengths, 12% higher tensile strength, and higher fatigue strength (by 21%) at 10^6 cycles for the micro alloyed steel.

COST ANALYSIS

Cost analysis is based on geometry changes and weight, modification in manufacturing process and the use of alternative material. The optimized geometry requires redesign and remanufacturing the forging dies used. The geometry parameters that influence machining and the final cost of the component include the increase of drilling process, because the drilled holes at the back of the crankshaft and the crankpin are redesigned to have larger diameters, and the bore at the back is modified to have more depth than the original bore.

The costs involved in study are separated in two elements of variable and fixed costs. Variable cost elements are the contribution to piece cost whose values are independent of the number of elements produced. Assumptions made for the cost analysis modeling are tabulated in Tables 2 and 3. The major difference between the assumptions in the case of hot rolled steel forging and micro alloy forging were those of the die life and material cost. In case of micro alloy forging, the quench and temper step was eliminated, resulting in cost savings.

Table 2 Manufacturing assumptions for a forged steel crankshaft weighing 14.787kg

<table>
<thead>
<tr>
<th>Factor</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Part Weight</td>
<td>14.787kg</td>
</tr>
<tr>
<td>Material</td>
<td>Hot Rolled Steel Bar (4130)</td>
</tr>
<tr>
<td>Die life (parts)</td>
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</tr>
<tr>
<td>Material Cost</td>
<td>Rs. 11/kg</td>
</tr>
<tr>
<td>Forging Impressions</td>
<td>2</td>
</tr>
<tr>
<td>Cavities/Impression</td>
<td>1</td>
</tr>
<tr>
<td>Maintenance</td>
<td>4%</td>
</tr>
<tr>
<td>Building Area</td>
<td>25,000 Sq Ft</td>
</tr>
</tbody>
</table>
Table 3 Manufacturing assumptions for a micro alloyed steel forging crankshaft weighing 14.787kg

<table>
<thead>
<tr>
<th>Factor</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Part Weight</td>
<td>14.787kg</td>
</tr>
<tr>
<td>Material</td>
<td>Micro Alloyed steel</td>
</tr>
<tr>
<td>Die life (parts)</td>
<td>20,000</td>
</tr>
<tr>
<td>Material Cost</td>
<td>Rs. 12.5/kg</td>
</tr>
<tr>
<td>Forging Impressions</td>
<td>2</td>
</tr>
<tr>
<td>Cavities/Impression</td>
<td>1</td>
</tr>
<tr>
<td>Maintenance</td>
<td>4%</td>
</tr>
<tr>
<td>Building Area</td>
<td>25,000 Sq Ft</td>
</tr>
</tbody>
</table>

CONCLUSIONS
1. Geometry optimization resulted in 10% weight reduction of the forged steel crankshaft, which was achieved by changing the dimensions and geometry of the crank webs while maintaining dynamic balance of the crankshaft.
2. Crankshaft geometry changes in this optimization stage required changing the main bearings in the engine according to the optimized diameters and using thrust bearings to reduce the increase of axial displacement of the crankshaft.
3. Using micro alloyed steel as an alternative material to the current forged steel results in the elimination of the heat treatment process. In addition, considering better machinability of the micro alloyed steel along with the reduced material cost due to the 18% weight reduction.

REFERENCES
INTER-COMPONENT FRICTION OPTIMISATION IN STAINLESS STEEL TORQUE-CONTROLLED EXPANSION ANCHORS FOR THE CONSTRUCTION INDUSTRY

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ABSTRACT
As one of the world's leading suppliers of fixings and fasteners, Rawlplug Limited operate within a highly competitive industry. In such a saturated market, despite the current economic climate, it is strategically beneficial to innovate. True to this theory, Rawlplug Ltd is currently developing specialist heavy-duty construction anchor products that will sit at the top end of the quality scale. The company's R&D department - with which the author is affiliated - now aims to develop a stainless steel torque-controlled expansion anchor capable of functioning in cracked and uncracked concrete. This would enable potential attainment of an 'Option 1' European Technical Approval (ETA); the highest level of safety certification. However, an obstacle stands in the way of this development. Stainless steel parts tend to fuse together when moving against one another under high loads, inhibiting the performance of expansion anchors. This paper details research wherein a range of lubricating coatings with varying coefficients of friction are applied at the critical interface in an attempt to optimise component interaction. Modified samples show improved performance, confirming the benefits of employing coated components in the assembly. Test analyses provide a foundation for further product development and possible ETA certification in the future.

INTRODUCTION
Fixings are products designed to facilitate the connection between two or more solid bodies, in order to create an assembled whole. The most frequently occurring example (relevant to this work), is the connection of steel to concrete in the construction industry. Other instances of fixings products (less relevant to this work) may be seen in the do-it-yourself (DIY) and small trade industries. These more lightweight products may alternatively be referred to as fasteners.

The structural assembly created by the use of a fixing generally consists of three elements; a fixture (the object to be fixed in place), a substrate (the base material), and the fixing to connect or fix the two. Figure 1 demonstrates this type of setup, showing a metal plate fixed to concrete by a torque-controlled expansion anchor. It is this type of fixing technology, and the optimisation thereof, which will form the focus of this particular work.

After exploring the background of the industry and product technology, the barriers to new product development are introduced. Subsequently the paper focuses on the test program designed to investigate performance optimization and the results, analysis and conclusions thereof.

CONSTRUCTION AND THE ECONOMY
There are three distinct markets for fixings products – construction, trade, and do-it-yourself (DIY). Of the three sectors, construction is the most significant in terms of both volume and value. Within this market, the range of technologies offered can be split in to a number of classifications, as EOTA has set out in Part 1 of the European Technical Approval Guideline (ETAG) [1]. This document lists these classifications as torque-controlled expansion anchors, undercut anchors, deformation-controlled anchors and bonded anchors. For further explanation, along with schematic representations of each technology, the reader should refer to the full ETAG document.

We will return to explore the technology of torque-controlled expansion anchors in more detail later in this
Firstly, however, it is necessary to familiarise oneself with the current economic factors playing a part in the fixings industry. Gilmore & Jordan [2] indicate that the contribution of construction to the UK economy is “about 6 per cent”. More precisely, the industry saw an output in the UK of £107.01bn in 2005, this being a 4.5% rise on the value of 2004 [3]. Recently, however, major economies including those of the UK and USA have been substantially weakened by the shockwaves of the economic crisis, and construction activity has slowed as a result. Gilmore & Jordan observe that in March 2008 the Construction Managers’ Index (which tracks activity in the UK’s housing, commercial and civil engineering markets) fell below 50 for the first time, indicating the start of a period of negative growth in the industry. Elsewhere a press release from the Construction Products Association [4] drew attention to Office for National Statistics (ONS) figures reporting the largest annual fall in commercial construction new orders since 1983. These worrying trends of construction inactivity on a global scale have an inevitable knock-on effect to the fixings industry. However, there is now some promise that government reinvestment in some of the major economies may promote extensive spending in construction. In the UK, the Government has committed in a 2008 document [5] to tackle “the historic backlog of under-investment in the country’s infrastructure”. According to the report capital spending in transport a decade ago was £2.9 billion, a figure which increased to £11.9 billion in 2008-09 with a planned £12.5 billion in 2009-10. Meanwhile the US President, Barack Obama, on the 17th February 2009 signed into law the “American Recovery and Reinvestment Act of 2009”. The Act [6] states that for investment in highway infrastructure “restoration, repair, construction and other activities”, $27.5 billion is to remain available through September 30, 2010. This constitutes part of the $111 billion total to be spent on infrastructure and science (see Figure 2) as part of the recovery effort.

We shall now move on to consider the background of this work, preceded briefly by details of author affiliation.

**AUTHOR AFFILIATION**

The work presented in this paper has been generated as part of a 24-month Knowledge Transfer Partnership (KTP) involving Glasgow Caledonian University and the R&D department of Rawlplug Limited – a leading manufacturer of fixings, located in Glasgow, Scotland.
The objectives of the partnership were as follows; 1) To identify and implement design improvements, 2) To manufacture previously outsourced products in-house, and 3) To carry out New Product Development (NPD) projects.

**SCOPE OF RESEARCH**

The work put forward in this paper falls under the latter of the aforementioned partnership objectives - NPD. Presented herein are research outcomes that contribute to the performance optimisation of a stainless steel version of Rawlplug’s current mild steel torque-controlled expansion anchor. As such, the product being developed (Figure 3) – whilst retaining the physical form and technological legacy of its predecessor – is new by virtue of the material from which it is manufactured and the associated new design challenges.

![Figure 3 – General form of the product under development, with main components & features](image)

In an attempt to overcome these challenges, development work involved the introduction of organic coatings to the product’s critical component interface – between the expansion sleeve and the tapered, conical section of the bolt (shown close-up in Figure 4). Three variants of the organic coating were sourced and applied to bolt samples. In order to assess the inter-component optimisation brought about by these modifications, four test sets were executed; three sets with coated parts, plus one with the unmodified part as a datum. Each set contained five individual samples. Therefore the overall test program spanned twenty individual tests.

![Figure 4 – Sleeve component (pre-expansion) resting at the lower end of the bolt cone](image)

**TORQUE-CONTROLLED EXPANSION ANCHORS**

It is first necessary to understand the technological background of the product family. This section will give a brief introduction to throughbolts (the relevant sub-category of torque-controlled expansion anchors), their functioning and the corresponding state-of-the-art in Rawlplug’s product range.

Throughbolts are so named because of their suitability for installation directly through the fixture and in to the substrate material (as shown in Figure 5). The bolt – pre-assembled with sleeve, nut and washer components – is hammered in to a pre-drilled hole, before tightening the hexagonal nut until a recommended installation torque level is achieved.

As highlighted in the ETAG, “Expansion anchors are anchored in drilled holes by forced expansion. A tensile force applied to the anchor is transferred to the concrete by friction and some keying between an expanded sleeve and the concrete” [1]. Rotation of the nut translates to linear motion of the bolt cone, causing the sleeve (which has become lodged against the hole wall during installation) to open, thus inducing “forced expansion” in the substrate. Subsequent load bearing capacity of the anchor depends heavily on the quality of product setting (expansion) during installation.

This ability to bear applied loads will also influence the failure mode of the anchor. Four modes of failure can typically be witnessed in torque-controlled expansion anchors; concrete cone, steel, pull-through and pull-out. Concrete cone failures occur when the cone of influence (Figure 6) – the conical volume of concrete under influence of the anchor expansion load – has a lesser load-bearing capacity than the anchor itself. Cracks thus propagate from the point of expansion to the substrate surface, typically resulting in a broken out conical section of concrete (Figure 7). Conversely, steel failures occur when the cone of influence possesses more load-bearing capacity than the anchor assembly. In this case one of the steel components will experience plastic deformation.
failures involve the complete anchor pulling out from the hole, typically at very low loads. The cause of this failure is insufficient friction and/or keying between the outer face of the sleeve and the substrate material, often caused by poor sleeve expansion. Pull-out failures must be avoided, as they can lead to the failure of the anchorage at dangerously low loads.

All four failure modes are summarised in Figure 10 where the resulting differences in performance are clear. Note the distinctive trend of high displacement at low load in the pull-out failure curve.

Moving on to a more product-specific focus, the current state-of-the-art in Rawlplug’s throughbolt range is the mild steel scant-shank version shown in Figure 11, details of which can be found in the company’s product catalogue [9]. Currently the product is available with thread diameters ranging from 6-24mm and in bolt lengths of 50-260mm. At the end of 2008 the mild steel product was granted an Option 7 European Technical Approval (ETA) [10], an accolade that is considered “a favourable technical assessment of its fitness for an intended use” [11]. The Option 7 approval indicates that the product has undergone the most thorough ETAG-based assessment outlined for uncracked concrete only.

The stainless steel version of the scant-shank throughbolt is being developed such that it can attain an Option 1 ETA. In this case the product assessment follows the most thorough test guidelines for performance in both cracked and uncracked concrete. An Option 1 ETA is one of the most highly regarded marks of quality available for European construction anchors. In order to perform to a sufficient and consistent level, the product will require optimised product setting.

Having explored Rawlplug’s throughbolt technology, the following section outlines the new challenges that were faced as a result of the change of material.
NEW PRODUCT DEVELOPMENT ISSUES

Major benefits of a stainless steel variant of a throughbolt include, firstly, its superior resistance to the corrosive action of atmospheric conditions. This allows the product to function in external and marine fixing scenarios. The second advantage is its enhanced value; due to the higher degree of specialism afforded to the product by its assessment against Option 1 ETA criteria. However, these eventual benefits depend on successful circumvention of the following design challenges.

Firstly, the design must be optimised to overcome the detrimental effects of galling; a phenomenon inherent in the use of stainless steel. Known to be a potential issue “with fasteners made of stainless steel…and other alloys which self-generate an oxide surface film for corrosion protection”, galling is a process wherein mating components weld together under high frictional loads [12]. In cases where galling occurs in throughbolts, the functioning of the product is compromised, often rendering it unfit for its intended purpose. The most common outcome of galling with this type of product is the prevention of full sleeve expansion (caused by the welding of the internal surface of the sleeve on the tapered face of the bolt). Evidently the resulting poor anchorage can lead potentially to pull-out failure. Therefore any testing herein should ideally indicate an absence of galling.

The second main challenge faced is the requirement that the product, in order to achieve the Option 1 approval, be designed to function favourably in both cracked and uncracked concrete. As is evident in Figure 12, cracked concrete can be thought of as any surface of a concrete member that is in a state of tension – for example, the underside of a concrete ceiling, sagging slightly under the influence of its own weight.

When cracked concrete tests are conducted in laboratory conditions, the performance of the product will be required to meet strict standards, despite hole diameters being widened by as much as 0.5 millimetres. In real terms this means that the level of expansion of the product during installation must be optimised. In cases where optimum expansion is not achieved the expander will fail to grip the internal walls of the hole, often leading to pull-out failure.

PROTOTYPES & TEST PROGRAM

This section outlines both the modifications made to the product and the test guidelines employed in order to assess their effect.

As indicated in previous sections, optimisation of the sleeve/bolt interface was required. Based on previous experience in Rawlplug’s R&D department it was hypothesised that galling could be eliminated by the introduction of a lubricating plastic coating between the part surfaces. The assumption was also made that the specific lubricating properties of the coating would have an effect on the extent to which friction was reduced, thus ultimately on product expansion performance.

In an attempt to ascertain the exact coefficient of friction (COF) required for optimum expansion, a test program was designed which would assess the varied lubricating effects of a range of coating compositions. Three sets of samples were processed, each with a different spray-applied coating:

1. Set C1 – Blue organic coating (COF = 0.15)
2. Set C2 – Blue organic coating (COF = 0.20)
3. Set C3 – Black organic coating (COF = 0.40)

It should be kept in mind that all components – bolt, sleeve, nut and washer – are manufactured from A4 grade stainless steel. The sole change being made is the application of one of the three coatings listed above.

Coated sample sets are displayed in Figure 13. The bolt cone was chosen for coating, in order that during expansion new plastic material would continuously be...
introduced at the component interface. Thus it was ensured that the coating effect would not be exhausted, leading to galling in the latter stages of the test.

Additionally to the three coated sets, a datum set made up of unmodified parts was assembled. This set and its samples are referred to herein as C0. The unmodified prototype appearance was as seen earlier in Figure 4.

Having at this stage obtained sets of the processed samples, it was necessary to design a test program for the assessment of product functioning during installation. It was decided that torque tests according to the ETAG would be employed to determine “the relation between the applied torque moment and the tension force in the bolt” [14]. The tension value achieved subsequently indicates the extent of sleeve expansion on the bolt cone.

Each torque test was set up according to Figure 14 (represented in real terms in Figure 15). Subsequently – after the throughbolt had been hammered to its specified embedment depth (68mm) – “the torque moment [was] applied with a calibrated torque wrench until it [could not] be increased further or at least to 1.3 T_{nut} respectively” [14]. (T_{nut} is the manufacturer’s recommended torque for the product - 50Nm in this case.) The torque wrench is shown in Figure 16, with the torque transducer, which records the applied torque moment in real-time, attached.

During torque application (and thus product expansion), load and torque data signals were fed from the load cell and torque transducer respectively to the Virtual Instrument (VI) software program. Data streams were then exported from the VI and analysed in Excel software, where data was processed in order to establish key performance indicators. Graphs showing the tension in the bolt as a function of the applied torque moment were then generated and analysed.

As suggested earlier in the paper, the process of set-up, testing (torque-application) and analysis was repeated for twenty individual tests, each contributing to the full test program.
each prototype’s suitability for its intended use. Next it is necessary to present the outcomes of this test program.

RESULTS AND ANALYSIS

This section presents results of the outlined test program, with initial performance analysis.

The first set of samples to be assessed in the torque test was the unmodified datum set – C0. A graphical representation of the relationship between bolt tension and applied torque moment for this set can be seen in Figure 17. (Note that in all graphical representations the bold horizontal line indicates the mean tension achieved at 65Nm.) This set, ultimately based on only four tests, due to a system error, returned an average achieved tension of 7.54kN at the 65Nm torque milestone. The mean variation of recorded tension values for the set – measured across the full range of torque – was 18.1%. Samples required approximately 2.8 nut revolutions to reach test completion.

The test curves for each individual C0 sample show a significant degree of fluctuation in the tension values as torque increases. Expansion forces in the hole (and the resultant tensile resistance) are rising and falling erratically as the nut is being tightened.

Moving on, set C1 was the next to be tested and the relevant test curves are presented in Figure 18. This set achieved an improved average tension of 9.58kN, whilst overall variance dropped to a more consistent 8.7%. It is evident from the noticeably closer spacing of the C1 curves (compared to C0) that consistency of expansion has improved. However, beyond 45Nm the curves begin to diverge once more.
Set C2’s performance curves are presented in Figure 19. Immediately the curve shapes suggest an increase in variance from the C1 set, with broader spacing and some clear separation of individual test curves. True to appearance, the variance value rises to 10.7%. However, this drawback is offset by a further increase in mean tension at 65Nm – 10.66kN is achieved in this instance.

Finally, set C3 (shown in Figure 20) achieves the highest mean tension – 11.15kN. However, curves again show an increased spacing, demonstrating that tension variance has risen again to 11.4%. Furthermore, divergence of the curves in this set appears to begin at torque values as low as 7Nm.

Having considered the test data for each individual test set, all results are summarised in Table 1. A number of trends can be drawn from this summary. Firstly, the recorded tension values increase sequentially from set C0 to C3. Secondly, after a substantial improvement (decrease) in variance from set C0 to C1, variance is then seen to increase for set C2 and subsequently C3 also. Thirdly, the final major trend sees a pattern developing in the number of nut revolutions required to reach product setting. This pattern appears to be inversely related to the variance trend, in that the revolutions increase substantially from C0 to C1, before decreasing steadily for subsequent sets.

Table 1 – Test program result summary

<table>
<thead>
<tr>
<th>Sample Set</th>
<th>Torque (Nm)</th>
<th>Tension (kN)</th>
<th>Overall variance</th>
<th>Revolutions required</th>
</tr>
</thead>
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<tr>
<td>C0</td>
<td>65</td>
<td>7.54</td>
<td>18.1%</td>
<td>2.8</td>
</tr>
<tr>
<td>C1</td>
<td>65</td>
<td>9.58</td>
<td>8.7%</td>
<td>5.4</td>
</tr>
<tr>
<td>C2</td>
<td>65</td>
<td>10.66</td>
<td>10.7%</td>
<td>4.8</td>
</tr>
<tr>
<td>C3</td>
<td>65</td>
<td>11.15</td>
<td>11.4%</td>
<td>3.1</td>
</tr>
</tbody>
</table>

The following section will discuss probable causes for these trends, as well as their possible implications.

DISCUSSION AND CONCLUSIONS

This section aims to provide an understanding of the trends outlined previously, especially with regards to the underlying product functioning.

The first trend showed a steady increase in mean tension values. Low tension in the C0 set was expected and is a probable outcome of the predicted galling between the sleeve and uncoated bolt cone. The suspected galling also coincides with the extensive fluctuation in the C0 test curves. All indicators suggest erratic expansion movements as the bolt cone is drawn through the sleeve in the hole. Moving on to set C1, it is no surprise then that the introduction of the lubricating coating results in increased tension. By reducing friction galling has been reduced or eliminated, thus enhancing expansion efficiency.

However, the most pertinent observation sees the extended increase of tension in sets C2 and C3. This suggests that the COF of 0.15 in coating C1 was in fact too low, reducing the setting tension beyond that of optimum performance. In simple terms, excessive lubricant had been introduced to the expansion interface. This causes the bolt cone to pull through the sleeve component too easily (i.e. at lower-than-optimum loads).

Therefore it can be concluded that the lesser quantities of integral lubricant in coatings C2 and C3 (COF 0.2 and 0.4 respectively) have brought the functioning at the expansion interface closer to the optimum scenario.

On a related note, the trend in nut revolutions reinforces the link between coating COF and expansion. Rotational motion of the nut on the thread translates to linear motion of the bolt along its axis. Therefore if fewer nut turns are required to set the product, this indicates shorter linear translation of the bolt and thus lesser levels of expansion.

In conclusion, the initial addition of an organic coating appears to eliminate the galling seen in set C0. Subsequently, it is clear that the COF of the coating is directly related to the tension achievable. The highest tension in this test series was achieved with a COF of 0.4. Further optimisation is required, experimenting (if possible) with higher COF values in similar coatings.

FURTHER WORK

As suggested previously, the most favourable expansion performance seen in this test program remains subject to optimisation. Despite achieving increased tension using higher COF values, the related trend of increasing variance is also evident. The cause of this reduction in consistency is not clear from this set of results. Possible causes are excessive expansion in some samples, or increased spinning/skewing of the sleeve component. It is also possible that increased smoothness of expansion and curve shape causes the inconsistencies of the concrete substrate to become more apparent upon comparison of individual tests. Whatever the cause, it is clear that variance at higher loads will have to be controlled to achieve the true optimum product performance. This is one possible line of investigation for future research.

A final additional consideration arising from this work centres on the possible occurrence of galling at the nut/thread interface. Functioning at this interface was outside the scope of this particular study. However, investigations in to the influence of component interaction at this interface are currently underway in Rawlplug Ltd’s test centre.
REFERENCES
NANO-INDENTATION OF MONOLAYER GRAPHENE SHEET USING
MOLECULAR DYNAMIC SIMULATIONS

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ABSTRACT

Graphene sheet has recently emerged as most exciting material system to study due to its high strength and rigidity, high room temperature electron mobility, and unconventional quantum Hall effect. Recent experiments show that the graphene sheet exhibits a Young’s modulus between 0.9 and 1.2 TPa. In this work a large-scale molecular dynamics (MD) simulation of the nano-indentation of a monolayer graphene sheet is performed using a spherical indenter to calculate Young’s modulus. An Adaptive Intermolecular Reactive Empirical Bond Order (AIREBO) potential is used for the carbon-carbon interaction. The MD simulation results for Young’s modulus of a graphene sheet are compared with experimentally calculated value. MD simulations results were found to be very much similar to the experimental values.

INTRODUCTION

Carbon is found in all living organisms and can be found in many allotropic forms. Generally, it is found in forms such as diamond, amorphous-carbon, or graphite. Carbon-carbon bonds are strong and stable. Graphite is one of the softest known materials while diamond is one of the hardest [1]. Figure 1 shows two allotropic forms of carbon, graphite and diamond, as well as their atomic structures, respectively.

Graphene is a monolayer “honeycomb lattice” [6] of a $sp^2$ bonded carbon atoms. It is the building block of all $sp^2$ bonded carbon nano-structures such as bucky-balls, nanotubes, and graphite. For example, graphene can be wrapped to form bucky-balls, rolled to form nanotubes, or stacked on top of one another, separated by van-der Waals interaction forces, to form graphite.

Graphene shows very interesting properties which make it a unique monolayer structure. Mechanically, it is the stiffest and strongest material known to mankind. It has a Young’s modulus of 1 TPa and a high intrinsic strength of 130 GPa [7], approximately 200 times stronger than structural steel [8]. Graphene also exhibits excellent electrical properties with very high current densities of the order of $10^8$ A/cm$^2$ [9]. More interestingly, they are materials with zero band gap, and the band gap can be controlled by controlling the width of the graphene sheet. Unlike optical properties of other monolayer structures, graphene has a high opacity absorbing 2.3% of white light [10]. Some potential applications for the single layer atom structure are pressure sensors, nano-resonators, nano-scale electronics, ultra capacitors, solar cells, etc.

Figure 1. Carbon has many allotropic forms and is well known for certain ones. (a) Piece of graphite [2]. (b) Structure of graphite [3]. (c) Piece of diamond [4]. (d) Structure of diamond [5].
PROBLEM STATEMENT

Recently in the experiment performed by Lee et al. [7], an AFM was used for indentation on monolayer graphene sheet membrane suspended over circular wells to measure the mechanical properties. Using reactive ion etching and nanoimprint lithography on a silicon (Si) substrate with a 300 nm SiO₂ epilayer, a 5-by-5 mm array of circular wells (diameters 1.5 µm and 1 µm, depth 500 nm) was patterned. Figure 2 shows images of graphene membranes on a Si substrate. Figure 2a shows different size circular wells, Figure 2b shows a graphene membrane adhering to the wall of a Si substrate, Figure 2c shows the indentation of a graphene membrane, and Figure 2d shows a punctured membrane.

During the experiment, graphene membranes were tautly stretched across the circular wells. Diamond tip cantilevers were used to study the mechanical properties by indentation. The AFM tip was positioned within 50 nm of the graphene membrane’s center [7]. Mechanical testing was performed at a constant displacement rate, followed by load reversal. The experiment was repeated using different indenter sizes, membrane diameters, displacement rates, and flakes [7]. In the experiments [7], two different diameters of circular wells were patterned on a Si substrate, one 1 µm and another 1.5 µm. Exfoliated monolayer graphene sheets were mounted on these holes as shown in Figure 2a. Different AFM tips with varying tip diameters were used to probe each flake. A load indentation curve was generated from the experiments and compared with the analytical solution given by [7].

Figure 2. (a) A graphene flake deposited on a Si substrate with circular wells 1µm and 1.5 µm in diameter. The circular well of area I is fractionally covered, area II is completely covered, and area III is punctured due to indentation. The scale bar is 3 µm. (b) An image from noncontact mode AFM of 1.5 µm diameter of a membrane adhering to the inside circular well of the Si substrate 2.5 nm. (c) The nanoindenter on suspended graphene membrane. (d) A punctured membrane viewed by AFM imaging [7].
The analytical solution is given by,
\[ F = \sigma_0^{2D} \left( \pi a \right) \left( \frac{\delta}{a} \right) + E^{2D} \left( q^2 a \right) \left( \frac{\delta}{a} \right)^3 \]  
(1a)
\[ q = \frac{1}{1.05 - 0.15v - 0.16v^2} \]  
(1b)
where \( F \) is the force applied to the graphene membrane by the indenter, \( \sigma_0^{2D} \) is the in plane pretension stress in the graphene that covers the hole on the Si substrate \( \delta \) is the indentation, \( a \) is the diameter of graphene sheet, \( E^{2D} \) is the in-plane Young’s modulus, and \( q \) is a dimensionless constant dependent on Poisson’s ratio \( v \). The unknowns \( \sigma_0^{2D} \) and \( E^{2D} \) in Equation 1a were determined [7] by least-square fitting the experimental data. Equation 1a is only valid when the indenter is in the center of the graphene, not eccentric. In the experimental study [7] the mean value of the in plane Young’s modulus \( E^{2D} \) was 342 Nm\(^{-1}\) with a standard deviation of 30 N·m\(^{-1}\). This value corresponds to the bulk value \( E \) of 1.0 TPa assuming the distance between the graphene sheets in graphite to be 3.343 Å.

Figure 3 shows 67 experimentally derived values of \( E^{2D} \) [7] from Equation 1a.

![Figure 3. Derived values of \( E^{2D} \) from Lee et al. [7].](image)

**MD SIMULATION**

MD simulation is used in this work to perform nanoindentation on monolayer graphene sheet. Due to the length-scale limitations of MD simulations, a reduced model is used compared to the actual graphene sheet dimensions in the experiment performed by Lee et al. [7]. MD simulation is more often used to simulate nanostructures since at this length-scale continuum mechanics tools are not applicable [11]. In MD simulation, atoms are assumed as lumped point masses which are under the influence of the interatomic potential \( \phi (r) \). The interatomic potential is an analytical expression derived either from experimental data or quantum mechanical calculations. The interactions are assumed in the form of interaction energy between two atoms as shown in Figure 4.

![Figure 4. The diagram shows the interatomic potential \( \phi (r) \) between two atoms. The force calculation \( F_i \) is shown as the derivative of the interatomic potential with respect to the distance \( r_i \) between the lumped point masses [11].](image)

Molecular dynamics is used to determine atom positions by solving Newton’s law of motion [11]

\[ m_i \ddot{r}_i (t) = F_i \]  
(2)
where \( m_i \) is mass, \( \ddot{r}_i \) is acceleration vector, \( t \) is time, and \( F_i \) is force vector. The force between atoms is calculated by the gradient of the interatomic potential after interaction energies have been calculated.

**MD MODEL AND METHODOLOGY**

The MD simulations are carried out using the Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) [12]. All simulations are carried out on a 96 CPU Linux cluster at the University of Arkansas, Fayetteville [13]. Figure 5 shows a MD simulation model containing 52873 atoms that is used to determine the applied load versus indentation of a simply supported circular monolayer graphene sheet. Atoms in the outer diameter (shown in red) have an in plane thickness of 15Å and are fixed. The remaining atoms (shown in green), with a diameter of 390 Å, are free and coupled to the external bath. The atoms in the outer diameter are fixed so the sheet doesn’t move in the z-direction. In the xy-plane additional roller constraints are used in the x- and y-directions to restrain the sheet from moving in those directions and rotating about the z-axis. Figure 5a shows the four regions that have these constraints and two areas are enlarged for clarity. A rigid indenter with a diameter of 150 Å is used to apply a load to the graphene sheet as shown in Figure 5b. This MD model is used for most of the simulations preformed in this paper.

The treatment of covalent bonds in LAMMPS is governed by a potential used to regulate intermolecular interactions. The adaptive intermolecular reactive empirical bond-order potential (AIREBO) [14] used in this work is defined by a sum over pairwise interactions, composed of covalent bonding (reactive
empirical bond-order (REBO)) interactions, LJ terms, and torsion interactions as follows:

\[ E = \frac{1}{2} \sum_i \sum_{j \neq i} \left[ E_{ij}^{REBO} + E_{ij}^{LJ} + \sum_{k \neq i, j} \sum_{l \neq i, j} E_{ijkl}^{\text{tors}} \right] \]  

(3)

The reason for using AIREBO is that it not only contains the REBO term, which is mostly used for carbon and hydrocarbon structures, but also contains the LJ term to mimic the van-der Waals interaction between graphene sheets. Although the LJ term is immaterial in case of monolayer graphene sheet, it can be used in the future to simulate graphite flakes with multiple layers of graphene sheets. The first term in Equation 3 is the reactive bond-order interaction proposed by Tersoff [14]

\[ E_{ij}^{REBO} = V_r^h + b_{ij} V_r^a \]  

(4)

where \( V_r^h \) is the repulsive and \( V_r^a \) is the attractive components of energy between atoms \( i \) and \( j \). \( b_{ij} \) is the bond-order term with complicated dependence on bond angles. The second term in Equation 3 is the intermolecular repulsion interactions created with a Lennard-Jones 12-6 potential as [14]

\[ E_{ij}^{\text{LJ}} = 4\varepsilon \left( \frac{\sigma}{r_{ij}} \right)^{12} - \left( \frac{\sigma}{r_{ij}} \right)^6 \]  

(5)

where \( \varepsilon \) has a unit of energy, and \( \sigma \) has a unit of length. The last term in Equation 3 is the torsion interaction potential which is primarily for focusing on network solids such as diamonds and small molecular fragments relevant to the chemical vapor deposition of diamond. This term is insignificant in this work. The parameters used in this work for AIREBO potential can be found in [14].

Before carrying out the MD simulation of nanoindentation a simple model is used to determine Poisson’s ratio for the AIREBO potential as explained in the Appendix.

The following two cases were considered in this paper using MD simulations and compared to Lee et al. [7]:

1. Varying Indenter Diameter.
2. Eccentric Indenter.

Figure 5. Molecular dynamic simulation of a simply supported circular monolayer graphene sheet before load is applied. The red atoms are fixed and the green atoms are free. (a) Top view of simply supported graphene sheet with roller constraints applied in the four rectangular regions. The constraints are applied to the right, left, top, and bottom of the graphene sheet to keep it from moving in the x-y plane and rotating about the z-axis. (b) Isometric view of simply supported graphene sheet with rigid spherical indenter.
RESULTS FOR VARYING INDENTER DIAMETER

Varying the diameter of the spherical indenter was a variable in the experiment performed by Lee et al. [7]. MD simulations in Figure 5 were carried out for one size of graphene sheet and four different indenter sizes. These analyses are used to determine if indenter size will change the Young’s modulus. The indenter diameters considered were 100 Å, 130 Å, 150 Å, and 200 Å. When indentation was performed, an increasing force was applied to the graphene sheet for 150000 time steps. Figure 6 shows the MD simulation calculations and the analytical solution in Equation 1a. A least-square fit of the MD simulation results is used to determine the in-plane Young’s modulus $E^{2D}$ in Equation 1a. The value of Young’s modulus $E$ is calculated by,

$$E = 0.335nm$$

where $0.335$ nm is the distance between graphene sheets in graphite. The diameter of the graphene sheet defined by variable $a$ in Equation 1a is the inner diameter or the section with free atoms (green atoms) shown in Figure 5. The results from Equation 1a show that an indenter diameter of 100 Å has a Young’s modulus $E$ of $1.07$ TPa. The remaining indenters of 130 Å, 150 Å, and 200 Å, have a Young’s moduli $E$ of $1.13$ TPa, $1.18$ TPa, and $1.28$ TPa, respectively. These results indicate that the Young’s modulus increases as the indenter diameter is increased. This may be due to an increase in contact area between the graphene sheet and indenter. This confirms that using smaller diameter indenters leads to more accurate values of the measure Young’s modulus.

![Graph showing MD simulation and analytical solution](image)

Figure 6. The diagrams represent the various indenter sizes used in the MD simulations. The monolayer graphene sheet is the same diameter for all cases, and the diagrams show the load-indentation depth curve comparing the MD simulation to the analytical solution. (a) The 100 Å diameter indenter has a Young’s modulus of $1.07$ TPa. (b) The 130 Å diameter indenter has a Young’s modulus of $1.13$ TPa. (c) The 150 Å diameter indenter has a Young’s modulus of $1.18$ TPa. (d) The 200 Å diameter indenter has a Young’s modulus of $1.28$ TPa.
RESULTS FOR ECCENTRIC INDUCTER

The spherical indenter was positioned within 50 nm of the membrane center in the experiment by Lee et al. [7]. As shown in Figure 7, the MD simulation considered the indenter diameter of 150 Å and the indenter eccentricity was 0 Å, 5 Å, 10 Å, and 15 Å. Figure 7a shows that the 0 Å indenter eccentricity (zero eccentricity) has a Young’s modulus of 1.18 TPa. Figures 7b, 7c, and 7d show that the 5 Å, 10 Å, and 15 Å indenter eccentricities have Young’s moduli of 1.17, 1.16, and 1.17 TPa, respectively. These results show that increasing eccentricity does not affect the Young’s modulus.

CONCLUSION

In this paper, MD simulation was used to simulate the indentation of monolayer graphene sheet. It was observed that by increasing the spherical indenter diameter, the measured value of Young’s modulus increases. The reason being an increase in the indenter diameter increases the contact area between the indenter and graphene sheet. The eccentricity of an indenter with a constant indenter size does not affect Young’s modulus. The measured values of Young’s modulus from the MD simulations are consistent with the experimental values determined by Lee et al. [7], which were between 0.9 and 1.2 TPa. Further work on understanding the influence of point defects in the graphene sheet and the interaction between the graphene sheet and the Si substrate is currently underway.

Figure 7. Load-indentation curve from MD simulation for 420 Å diameter monolayer graphene sheet and 150 Å diameter indenter with four indenter eccentricities. Indenter with eccentricity of (a) 0 Å, has a Young’s modulus of 1.18 TPa. (b) 5 Å, has a Young’s modulus of 1.17 TPa. (c) 10 Å, has a Young’s modulus of 1.16 TPa. (d) 15 Å, has a Young’s modulus of 1.17 TPa.
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APPENDIX: POISSON’S RATIO CALCULATIONS FOR AIREBO POTENTIAL

The purpose of this appendix is to calculate Poisson’s ratio of monolayer graphene sheet using a MD graphene sheet. Poisson’s ratio is required to determine the dimensionless constant $q$ in Equation 1b, which is used to determine Young’s modulus. The monolayer graphene sheet in Figure A.1 consists of 13098 atoms (not shown). Carbon-carbon interaction is defined by the adaptive intermolecular reactive empirical bond-order (AIREBO) potential. The vertical left hand boundary of the sheet, shown in Figure A.1, has roller constraints in the $x$-direction and is free to move in the $y$-direction. The atoms at the right hand vertical boundary are pulled uniformly in the $x$-direction with a very small velocity $v_x$ of 0.5 Å/ps. Atom coordinate data was recorded from the middle section in both the $x$- and $y$-directions. From this data, using $x_1$, $x_2$, $y_1$, and $y_2$, the longitudinal and lateral strains were calculated. The small longitudinal strain $\varepsilon_x$ is calculated using

$$\varepsilon_x = \frac{\text{Change in Length}}{\text{Original Length}} = \frac{x_2 - x_1}{x_1} \quad (A.1)$$

and small lateral strain $\varepsilon_y$ is given by

$$\varepsilon_y = \frac{\text{Change in Length}}{\text{Original Length}} = \frac{y_2 - y_1}{y_1} \quad (A.2)$$

Poisson’s ratio is given by

$$\nu = \frac{\text{Lateral Strain}}{\text{Longitudinal Strain}} = \frac{\varepsilon_y}{\varepsilon_x} \quad (A.3)$$

The Poisson’s ratio was determined by calculating the lateral and longitudinal strains from the MD analysis as shown in Figure A.2. The longitudinal strain $\varepsilon_x$ and lateral strain $\varepsilon_y$ are calculated at each time step. Poisson’s ratio was determined to be 0.166 as shown in Figure A.2. In the experiment by Lee et al. [7], Poisson’s ratio for graphite in the basal plane was taken as 0.165. The MD simulation and experimental values are approximately the same.
Figure A.1. Diagram showing the monolayer graphene sheet with constraints used to calculate Poisson’s ratio. The left hand vertical boundary has roller constraints, and the right hand vertical boundary has a prescribed small velocity applied in the positive x-direction. These constraints allow the sheet to uniformly stretch in the x-direction and uniformly contract in the y-direction, allowing for the calculation of Poisson’s ratio.

Figure A.2. Poisson’s ratio $\nu$ versus longitudinal strain $\varepsilon_x$ based on MD simulation.