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In-silico Wear Prediction for Knee Replacements - Methodology and Corroboration

1 Abstract:

2 The capability to predict *in-vivo* wear for knee replacements is a very valuable pre-clinical analysis
3 tool for implant designers. Traditionally, time-consuming experimental tests have been the principal
4 means of investigating wear. More recently, computational models have offered an alternative.
5 However, the robustness and applicability of these models has not been demonstrated across a
6 range of designs and test conditions, and several different formulas are in use for estimating wear
7 rates. This gave limited confidence in the predictive power of these *in-silico* models.

8 In this paper, a new high-speed model for evaluating adhesive/abrasive wear rates is described, and
9 corroboration of this model with a wide range of different experimental wear tests reported in the
10 literature for different implant designs and loading conditions on different test platforms is
11 performed.

12 The number of different tests we have corroborated gives greater confidence in the performance of
13 this new wear-assessment tool, and allows us to provide better estimates of the wear 'constants'
14 used in computational models. The high speed of this new model allows us to evaluate a range of
15 alternative algorithm formulations, and so demonstrate the importance of including terms such as
16 the influence of cross-shear (CS). We conclude that the CS-based 'A/A+B' wear model offers the best
17 predictive power compared to other existing wear algorithms. Because simulation times are reduced
18 to only a few minutes, these models are ideally suited to large-volume 'design of experiment' or
19 probabilistic studies (which are essential if pre-clinical assessment tools are to begin addressing the
20 degree of variation observed clinically and in explanted components).

21

1 Introduction:

2 An implanted Total Knee Replacement (TKR) is a complex system, and there are many potential
3 pathways to failure. Nonetheless, amongst these, mechanical wear of the polyethylene components
4 continues to attract considerable attention from implant designers and clinical professionals.
5 Unfortunately, wear cannot currently be readily measured *in-vivo*, so wear assessment must be
6 performed using simulators. Historically these have been experimental tests (e.g. [1, 2]), as the
7 causal mechanics of wear have not been quantitatively described. However, performing these tests
8 involves considerable time and expense, and questions remain as to whether experimental tests are
9 capturing all the relevant *in-vivo* conditions, and the influence of variability from knee to knee post-
10 implantation.

11 The specific need exists for pre-clinical wear prediction tools to avoid these limitations of
12 experimental simulator testing. Computational platforms can deliver high-speed, low-cost
13 simulations; designed to either replicate *in-vitro* experimental mechanical conditions or else directly
14 simulate *in-vivo* conditions. However, since these models must explicitly model the physics of wear,
15 it is essential that they are corroborated with data collected using real-world assessments (either
16 experimental or clinical). To-date, *in-silico* wear models have been tuned to and compared with only
17 small experimental datasets, either by using published pin-on-disc (POD) data, e.g. in [3, 4], or else
18 by directly comparing against TKR wear simulator results, e.g. [5, 6]. Whilst these studies
19 demonstrate the value of *in-silico* methods in individual cases, they cannot robustly corroborate
20 across a range of test conditions.

21 Further, there exist a number of different proposals for how wear should be analytically modelled -
22 each using different mathematical equations to formulate wear algorithms. The original baseline
23 model proposed by Archard [7] was first applied to UHMWPE wear by Maxian et al [8]. It is designed
24 purely to model adhesive/abrasive wear damage (neglecting other mechanisms such as 3-body

wear), and uses a very simple proportional relationship to estimate the localised wear depth at any point on the contacting surfaces:

$$\text{Wear Depth, } H \text{ (mm)} = \text{wear factor, } K_w \text{ (mm}^3\text{/N.m)} \times \text{Contact Pressure, } p \text{ (N/mm}^2\text{)} \times \text{Sliding Distance, } S \text{ (m)}$$

However, experimental observations have demonstrated a strong path-dependence for wear rates [4, 9]. Simple uni-directional or bi-directional sliding produces minimal wear, whereas a high degree of variation in the direction of sliding greatly increases the wear rate. The measure of this variation in direction is termed 'cross-shear' (CS). In light of this observation wear models have been proposed which predict greater wear as the degree of CS is increased [3, 4, 10, 11]. Generally, these involve a modification of the above formula, to make the wear-factor K_w a function of CS. More recently, the assumption that wear increases uniformly with increasing contact pressures has been challenged; studies by Mazzucco et al [12], Ernsberger et al [13] and Kang et al [14, 15] have all suggested that the traditional model (where wear is directly proportional to contact pressure) is not correct; however, these tests were all performed in the simpler domain of POD tests, where geometry is not a confounding factor, and contact pressure is (ideally) constant across the articulating surface. How applicable these conclusions are for more the complex geometries, kinetics and kinematics of TKR wear is a matter of ongoing debate. A major obstacle in comparing and testing these different proposals for wear algorithms is that there is often limited experimental data to base the formulae on, and small numbers of trials (often in the limited domain of POD tests) cannot provide sufficient grounds to explore the differences between the various algorithms proposed. Therefore, the need exists to apply these algorithms across a wider range of experimental TKR tests to corroborate their performance on a larger scale.

Method:

1 *In-silico* wear prediction has previously been demonstrated using finite-element (FE) based
2 computational methods [5, 10, 16, 17]. For improved computational performance in this new
3 generation of models, fast rigid-body simulations have been derived from extant FE models [18].
4 Within the domain of FE modelling, rigid-body models have been demonstrated to give comparable
5 results to deformable models at a fraction of the computational cost [19]. These test-cases are based
6 upon ‘true’ dynamic simulations using multi-body dynamics (MBD) software (MSC.ADAMS, MSC
7 Software Corporation). Previous studies have demonstrated that rigid-body FE models and MBD-
8 based models give similar results for both deterministic and probabilistic analyses [18, 20].

9 A discretised spring-bed distributed across the tibial component articulating surface is used to model
10 tibiofemoral contact conditions, with spring properties tuned to match experimental contact
11 pressures [21, 22], essentially forming a ‘bed of springs’ elastic-foundation relating contact force to
12 interpenetration distance (as reported in other studies [23]). This contact also included a ‘coulomb’
13 friction model, with coefficients selected to be generically representative of TKR test conditions [24].

14 The initial wear predictions used with this model are based on standard algorithms widely reported
15 in the literature; the baseline Archard/Lancaster sliding-distance model [7] (without CS), and other
16 algorithms including CS (e.g. ML/AP [10], A/A+B [4], and σ^* ‘crossing intensity’ [3]). Alongside these
17 existing formulations, alternative arrangements have been included to explore the effect of
18 excluding contact pressure (CP) from the wear model [12-14].

19 Twenty-two different experimental tests were selected, sourced from the public literature and
20 proprietary test data, where the polyethylene tested was ‘conventional’, i.e. with minimal or no
21 cross-linking as part of the manufacture process, to ensure that the tests would be broadly
22 comparable. Implant geometry was acquired from manufacturers or reverse-engineered. Results for
23 a range of kinematics under displacement-control for the PFC sigma (fixed and mobile bearing
24 designs) and LCS were sourced from [1, 25]. These implants were also tested under ISO 14243-1
25 force-control [26]. Results for the NexGen CR implant were corroborated under force-control [5, 27]

1 and displacement control [28]. Additional implants included were the Vanguard PS under ISO force-
2 control [29], and Triathlon CR under displacement control [30]. Proprietary unpublished test data
3 was also used to corroborate semi-constrained & unconstrained design variants of the PFC sigma
4 under displacement-controlled conditions. Finally, tests of femoral components against ‘flat’
5 polyethylene surfaces using displacement control [31] were included to corroborate the wear
6 algorithms across a wider range of contact pressures & areas *in-vitro*. The full list of test-cases is
7 summarised in table 1. Note that because of the number of tests, it is not possible to include the full
8 set of test-conditions in this paper for every case. In each model, the same procedure was followed;
9 component positioning, allowed motions, spring constraint (where applicable), input loading
10 profiles, etc were matched to the reported test conditions in the literature. where these conditions
11 were not stated, and where the original investigators could not be successfully contacted for further
12 clarification, ‘generic’ test conditions were imposed (e.g. assuming a 60-40 M-L load split [32], using
13 a representative friction co-efficient of 0.04 [24], and adjusting the model configuration according to
14 a typical set-up for the test machine being used; i.e. replicating the standard mechanical
15 configurations for Instron, ProSim, or AMTI simulator rigs, as available from the manufacturers).
16 Readers are referred to the respective references for more details on individual test cases.

17 Wear rates reported in mg were converted to mm³ using a density of 0.93mg/mm³. To limit
18 computational times for this exploratory study, volumetric wear rate for each case was calculated
19 based on a single-cycle; published experimental and computational long-term studies demonstrate
20 that whilst linear wear depth rates may vary over time, volumetric wear is reasonably linear [5].

21 Once all the necessary experimental configuration data had been obtained for these tests (e.g.
22 implant geometry, loading input waveforms, spring restraint setup, available degrees of freedom,
23 etc.) the tests were simulated *in-silico* using the fast rigid-body model, and predicted wear was
24 evaluated for each of the proposed wear formulations included in the model. The computationally-

derived rates were then compared to the reported experimental wear rate (with error levels, where available). This allowed the predictive power of different wear algorithms to be compared directly.

Results:

All of the test-cases were simulated successfully and were post-processed to evaluate predicted wear using the different algorithms. The volume of data generated is considerable, so wear contour maps are not compared here; only the baseline volumetric wear rate for each model using each algorithm is reported. Wear constants were based on values reported in the literature; however this new larger data-set gives a better basis for selecting a wear constant, and new wear constants are proposed based on the results of this study for some commonly-used wear models.

Figures 1-5 show correlation plots for a few of the selected models. It is immediately clear from the results that the baseline Archard model has very limited predictive power to assess TKR wear (Figure 1). By comparison, every variation of wear algorithm which includes some representation of CS has a much greater predictive power (typically R^2 of 0.5 – 0.6 – e.g. see A/A+B model in Figure 2). Considering these CS models, there are several important observations. First, the inclusion or exclusion of contact pressure as a proportional term within the algorithm does not consistently or considerably alter the predictive power of the model for this particular set of test-cases. Second, the precise 'definition' (i.e. mathematical formulation) of CS used is of secondary importance compared to the decision to include or exclude a CS metric – the relative difference between alternative CS-based models is less than the difference between models with and without CS (compare Figures 2 & 3). Again, the treatment of CP within the algorithm also appears to be of secondary importance; both models with a proportional-CP term, and with no CP term, have similar predictive power for this set of test cases, provided that a CS metric is included (compare figures 3 & 4); the models including a proportional CP term appear slightly stronger, however the role of contact-pressure in

wear mechanics remains unclear – a plot of wear rate vs. cycle-averaged CP reveals no noteworthy correlations (see figure 5). Despite these uncertainties, it is possible to ‘rank’ the performance of the different CS algorithms for this particular test-case set. Based on this set of test-cases, the A/A+B wear model proposed by Turell [4] appears to be marginally the strongest predictor of *in-vitro* wear (Figure 2).

Previously, the reported empirical wear constants used in mathematical models of wear have been based on limited data-sets (e.g. a small sample of POD test results [4]). Based on this study, regression-fitting techniques were used to provide a set of wear constants for the different models, tuned to this group of test-cases, for use by other researchers to improve their TKR wear predictions in-future. This has two advantages; the constants are directly based on TKR tests, rather than derived from POD or THR tests (removing a potential confounding factor) and the values have been assigned based on this larger ‘training’ data set. The values suggested for the different models are listed in table 2.

Discussion:

It is not possible to speak of an empirically-defined model as being ‘correct’, since it has no direct analytic derivation. Therefore, the relevant question is: which model appears to offer the greatest predictive power? Previously, published studies have only corroborated with individual experimental tests, and so the performance of these models is not well-understood. Undertaking a more comprehensive corroboration requires multiple simulations from different sources, which necessitates a much faster modelling platform than intricate deformable-FE models; the rigid-body models demonstrated in this study require much lower simulation times (on the order of minutes, rather than hours). The combination of *in-vitro* & *in-silico* wear prediction methods corroborated together provides the fullest, most powerful toolset for pre-clinical analysis of TKR wear. *In-silico*

1 studies in isolation are subject to suspicion as long as there is no consensus on the precise causal
2 mechanics of wear. But *in-vitro* studies alone cannot provide the same range and volume of
3 information as can be quickly and efficiently evaluated computationally.

4 Of course, there are important limitations to these studies; the simulation can only perform well if
5 the underlying behaviours are modelled correctly, so the actual mechanical conditions must be
6 accurately captured to set a 'benchmark' for corroboration. A pertinent observation from the
7 multiple test-case corroboration is that there is considerable variability in the experimental results
8 reported in the literature (both within, and especially between, different research centres). This
9 could be due to variations in standard experimental procedure (e.g. whether wear is reported for
10 the counter-face or not, whether secondary axes such as M-L translation or V-V rotation are fixed or
11 free, etc) or simply due to unintentional errors (component mal-positioning, measurement
12 tolerances, etc). This is a serious confounding factor in attempting to provide a more exhaustive
13 corroboration; the 'noise' due to experimental variability masks the finer influence of the choice of
14 wear algorithm. This can be mitigated to some extent if all the particulars of the experimental
15 procedure are fully reported (and so can be recreated in the computational model), and if tolerances
16 on *in-vitro* uncertainty are reduced to a minimum. Only by corroborating with a 'tighter' set of
17 experimental test results will it be possible to determine with greater confidence which is the most
18 appropriate empirical algorithm for wear prediction (i.e. the best formulation for CS, the true
19 influence of contact pressure & area, etc).

20 Nonetheless, this study has clearly demonstrated that CS of some form must be an integral part of
21 any wear algorithm if it is to have useful predictive power. The simple Archard/Lancaster sliding
22 distance models have clearly been shown to be limited in their applicability – whilst it is possible to
23 'tune' an empirical Archard wear constant to match for a limited range of kinematic conditions, this
24 model clearly breaks down when a wide range of kinematics and different designs are considered, as
25 in the present investigation.

1 The present study compared models with and without a proportional term for contact pressure, in
2 light of current debates about the role of CP in polyethylene wear. The results are not conclusive;
3 both families of models had comparable predictive power; with neither showing a clear advantage.
4 This may indicate that the range of contact pressures encountered in standard TKR wear tests does
5 not vary sufficiently for the influence to become apparent, or that there are antagonistic factors
6 which have a confounding influence (e.g. increased articular conformity will reduce CP, but may also
7 be influencing debris transport, lubrication, etc). Again, ultimately the best way to resolve this issue
8 is with a greater number of well-defined, targeted corroborations between *in-vitro* and *in-silico* wear
9 analysis platforms.

10 There are many possible improvements and extensions to the models presented here; besides the
11 challenge of accurately capturing experimental conditions, adaptive models could be used to
12 investigate long-term wear for each test case(as in [5]). Probabilistic methods could be used to
13 attempt to capture the experimental uncertainty *in-silico*. As understanding of wear mechanics
14 improves, the wear algorithms could be customised to different combinations of articulating
15 materials (e.g. different UHMWPE grades). All these tests are for gait-simulation (mostly based on a
16 derivative of the ISO standard) it would be beneficial and informative to extend this to include a
17 much wider range of activities with more varied loading; however this would of course require
18 extensive corresponding experimental test data. Corroborating within a single framework for a wider
19 range of implant designs, simulator configurations, lubrication conditions, materials and loading
20 regimes will all ultimately play a part in augmenting our holistic understanding of TKR wear.

21 This study has aimed to illustrate the valuable role *in-silico* models can play in better exploring and
22 refining fundamental concepts regarding the causes of polyethylene wear in TKR. It demonstrates
23 that the current generation of CS-based empirical wear models have useful predictive power when
24 corroborated with *in-vitro* experiments and are able to qualitatively rank the wear performance of
25 different designs under different loading regimes, but there is room for further refinement in our

current understanding of wear, and hence also in the modelling of wear. Most importantly, it is apparent that the only way to refine and improve our understanding of wear is through more and better corroboration between both computational and experimental approaches, to exploit the unique strengths of both domains. By doing so, the pre-clinical analysis tools used for wear prediction in the future will offer designers a richer, faster, more powerful, and more accurate insight into the causes of wear in TKR.

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Source(s)	Implant(s) (PE derivative)	Inputs (forces & kinematics)
<i>McEwen et al [1]</i>	<i>Sigma FB & RP; LCS (GUR1020 & 1050)</i>	<i>Displacement (various kinematics) & ISO 14243-1 (Force) Gait</i>
<i>Galvin et al [31]</i>	<i>Sigma femoral on flat PE (GUR1020)</i>	<i>Displacement-driven Gait (various levels of kinematics)</i>
<i>Knight et al [5]</i>	<i>NexGen CR (GUR1050)</i>	<i>ISO-derivative Gait</i>
<i>Cottrell et al [27]</i>	<i>NexGen CR (GUR1050)</i>	<i>ISO 14243-1 (Force) Gait</i>
<i>Muratoglu et al [28]</i>	<i>NexGen CR (GUR1050)</i>	<i>ISO-derivative Gait</i>
<i>Williams et al [30]</i>	<i>Triathlon (GUR1020)</i>	<i>ISO-derivative Gait</i>
<i>Haider et al [26]</i>	<i>Sigma FB & RP (GUR1020)</i>	<i>ISO 14243-1 (Force) Gait</i>
<i>Haider et al [29]</i>	<i>Vanguard PS (GUR1050)</i>	<i>ISO 14243-1 (Force) Gait</i>
<i>Proprietary unpublished data</i>	<i>Sigma FB CVD/PLI (GUR1020)</i>	<i>Displacement-driven ISO-derivative & high-kinematics gait</i>
<i>Proprietary unpublished data</i>	<i>Sigma femoral on flat PE (GUR1020)</i>	<i>ISO-derivative; High & low levels of axial load & IE rotation</i>

Table 1: Listing of test-cases used for corroboration, with references where applicable

1

Wear Depth Formulation	Historical (Legacy) Constant, K_w	Revised Constant, K_w (based on test-cases)	Model predictive power with new constant (R^2)
Archard $H = K_w \cdot p \cdot S$	$2.64 \times 10^{-7} \text{ mm}^3/\text{N.m}$	$2.0 \times 10^{-7} \text{ mm}^3/\text{N.m}$.12
Sliding distance $H = K_w \cdot S$	-	$1 \times 10^{-6} \text{ mm/m}$.04
ML/ML+AP $H = K_w \cdot CS \cdot p \cdot S$	$3 \times 10^{-6} \text{ mm}^3/\text{N.m}$	$2.7 \times 10^{-6} \text{ mm}^3/\text{N.m}$.58
A/A+B $H = K_w \cdot CS \cdot p \cdot S$	$3 \times 10^{-6} \text{ mm}^3/\text{N.m}$	$3.3 \times 10^{-6} \text{ mm}^3/\text{N.m}$.60
σ^* $H = K_w \cdot (\sigma^*)^2$	-	$1.1 \times 10^{-5} \text{ mm}^3/\text{N.m}$.29
ML/ML+AP (no CP) $H = K_w \cdot CS \cdot S$	-	$1.43 \times 10^{-5} \text{ mm/m}$.54
A/A+B (no CP) $H = K_w \cdot CS \cdot S$	-	$1.8 \times 10^{-5} \text{ mm/m}$.49

2 *Table 2: Summary of current and suggested wear constants for different algorithm formulations.*

3

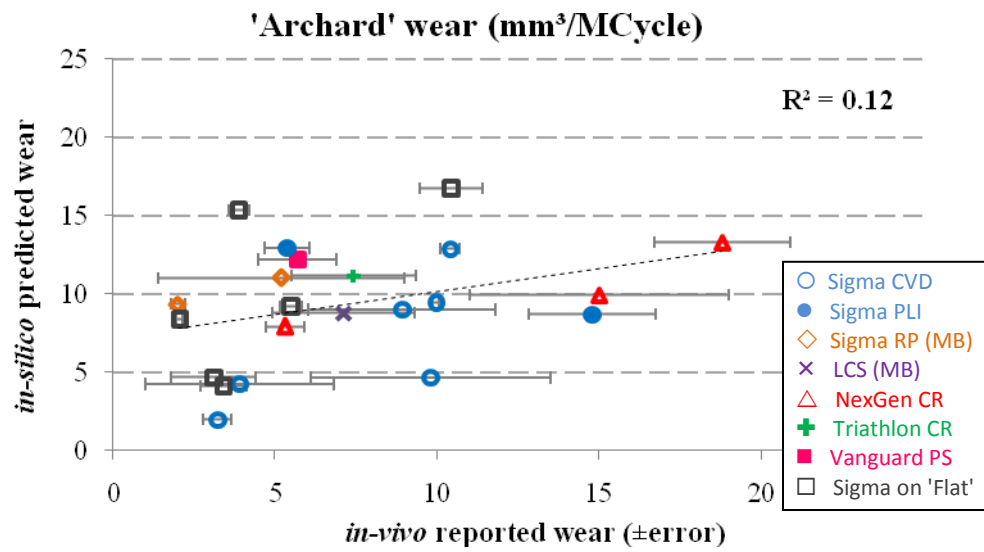


Figure 1. Experimental wear vs. wear predicted using 'Archard' algorithm.

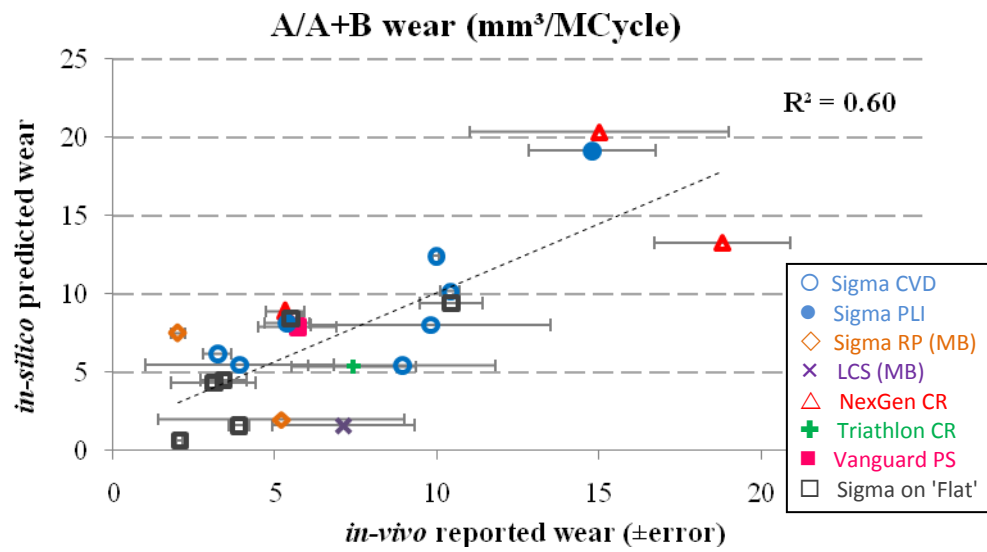


Figure 2. Experimental wear vs. wear predicted using 'A/A+B' algorithm.

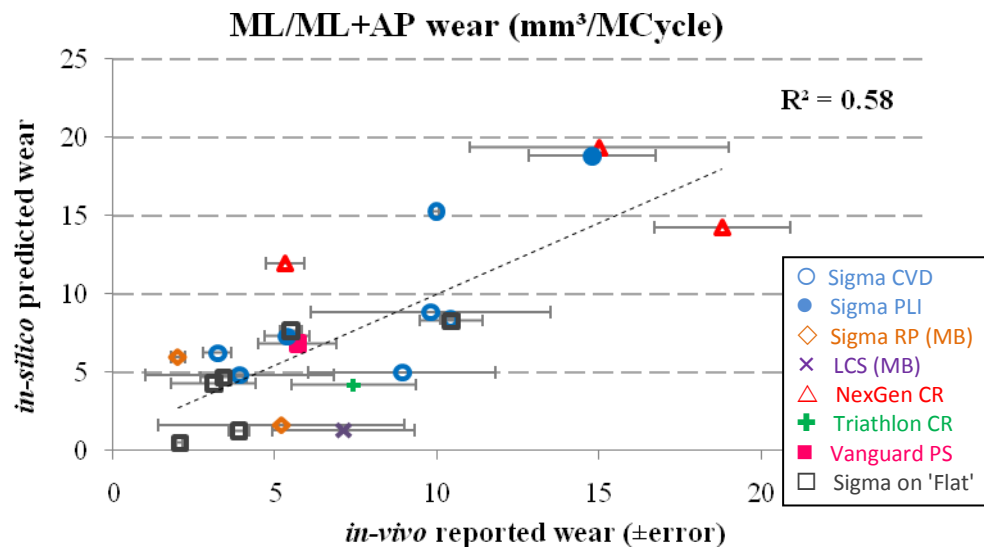


Figure 3. Experimental wear vs. wear predicted using 'ML/ML+AP' algorithm.

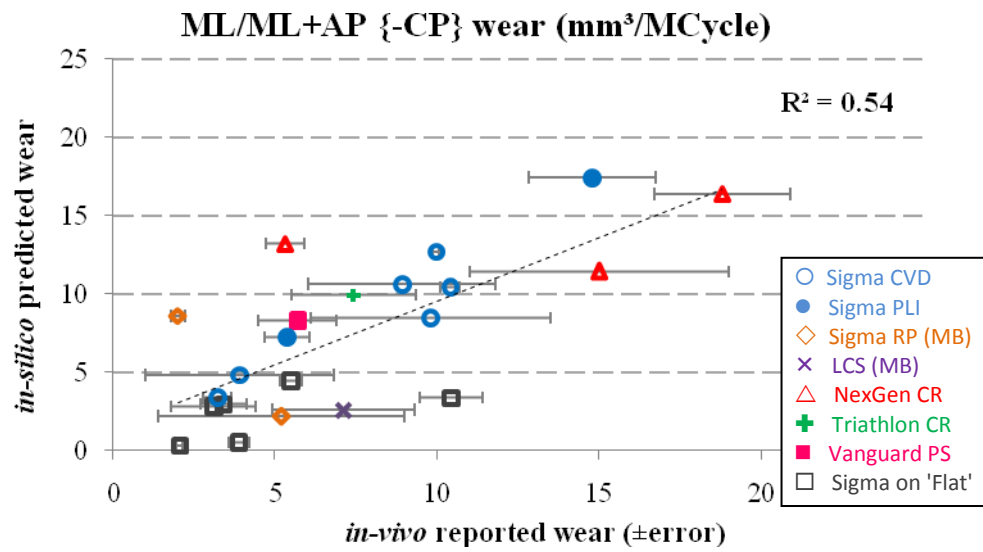


Figure 4. Experimental wear vs. wear predicted using 'ML/ML+AP' algorithm (without CP).

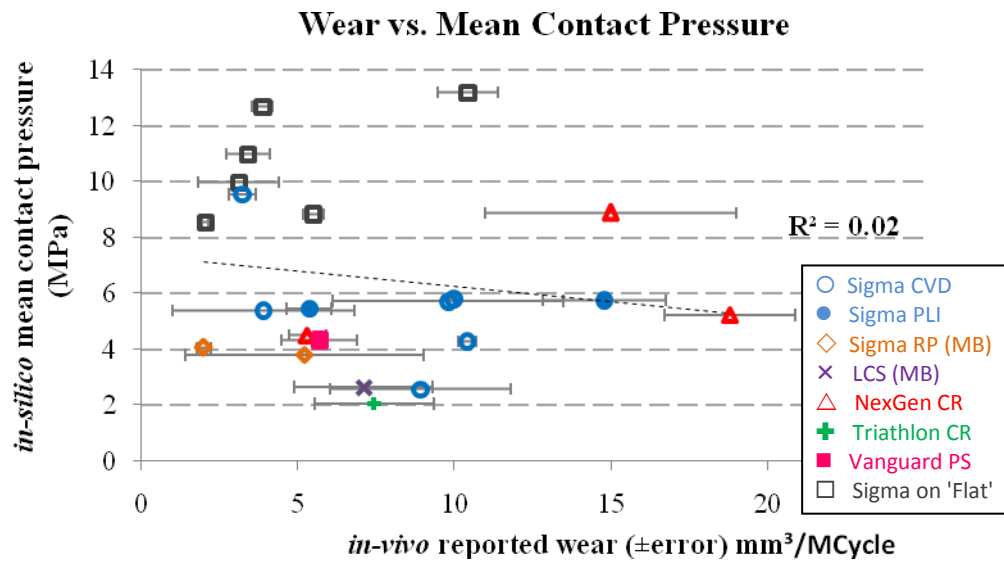


Figure 5. *in-vitro* wear vs. cycle-averaged contact pressure, showing no strong correlations.