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The influence of cross shear and contact pressure on the wear of UHMWPE-on-PEEK-OPTIMA™ for use in total knee replacement

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ABSTRACT

PEEK-OPTIMA™ polymer is being considered as an alternative material to cobalt chrome in the femoral component of total knee arthroplasty to give a metal-free knee replacement system. Simple geometry pin-on-plate wear simulation can be used to systematically investigate and understand the wear of materials under many different conditions. The aim of this study was to investigate the wear of UHMWPE-on-PEEK-OPTIMA™ under a range of contact pressure (2.1–80 MPa) and cross-shear ratio (0–0.18) conditions.

With increasing contact pressure, there was a trend of decreasing UHMWPE wear factor with a significant difference ($p<0.001$) in the wear factor of UHMWPE under the different contact pressure conditions of interest. Under uniaxial motion (cross-shear ratio = 0), the wear of UHMWPE was low, introducing multi-axial motion increased the wear of the UHMWPE. There was a significant difference ($p<0.01$) in the wear factor at different cross-shear ratios however, post hoc analysis showed only the study carried out under unidirectional motion to be significantly different from the other conditions.

With varying contact pressure and cross-shear ratio, the wear of UHMWPE against PEEK-OPTIMA™ polymer showed similar trends to previous studies of UHMWPE-on-cobalt chrome.

1. Introduction

Total knee replacement is a highly successful procedure with >100,000 procedures carried out in the UK annually and an estimated survivorship >90% at 10 years (National Joint Registry, 2022). However, with 1 in 5 patients dissatisfied with their outcome (Bourne et al., 2010), further research into knee replacement materials, geometry and surgical positioning is required. PEEK-OPTIMA™ polymer (PEEK) (Kurtz and Devine, 2007) has been considered as an alternative to cobalt chrome in the femoral component of total knee replacement, when coupled with an all-polymer tibial component, the knee system would be metal free and with a reduced weight compared to conventional materials. The modulus of the PEEK femoral component is closer to bone than cobalt chrome which may reduce stress shielding (Cowie et al., 2016a; Rankin et al., 2016; Meng et al., 2018; Du et al., 2018; de Ruiter et al., 2020, 2021). There is also a growing concern about metal sensitivity (Granchi et al., 2008) and the use of metal, particularly cobalt and chromium in the body which could be removed by implanting an all-polymer joint. Prior to clinical adoption, new implant materials must be rigorously studied in the laboratory (Jennings et al., 2012; Cowie and Jennings, 2021). Experimental wear simulation studies of the PEEK-on-UHMWPE bearing couple have previously been carried out in both whole joint simulation (Cowie et al., 2016a, 2023; Zhang et al., 2023) and simple geometry (East et al., 2015; Baykal et al., 2016; Cowie et al., 2019, 2020; Chamberlain et al., 2019; Heuberger et al., 2021) and have shown an equivalent rate of wear ofUHMWPE against PEEK and metal counterfaces. The focus of this study was to better understand the wear performance of the UHMWPE-on-PEEK bearing couple under a wider range of contact pressure and cross shear conditions through a series of studies carried out in simple geometry.

Simple geometry pin-on-plate wear simulation allows individual variables such as contact pressure, cross-shear ratio, sliding distance, lubricant, test environment and materials to be isolated and investigated systematically (Minakawa et al., 1998). The wear of UHMWPE-on-metal bearing couples has been investigated extensively to differentiate between different polyethylene compositions, molecular structure, cross-linking, sterilisation and for inputs to computational models. Studies have shown polyethylene wear to be dependent on both applied contact pressure and cross-shear ratio when articulating against a metallic counterface (Kang et al., 2008a, 2008b; Liu et al., 2011;

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Abdelgaied et al., 2013, 2018; Wang, 2001). Contact pressures from 2 to 80 MPa have been investigated and have shown a trend of decreasing wear factor with increasing contact pressure for polyethylene-on-metal (Liu et al., 2011; Abdelgaied et al., 2011, 2018). Cross-shear ratio is a description of the multidirectionality of the motion, and wear factors of polyethylene under multidirectional motion can be up to 10-times that of unidirectional motion (Kang et al., 2008a; Abdelgaied et al., 2011, 2013, 2018; Wang, 2001; Bragdon et al., 1996).

In the investigations of the UHMWPE-on-PEEK bearing couple carried out to date, a limited range of kinematic conditions have been studied, (East et al., 2015; Baykal et al., 2016; Cowie et al., 2019; Chamberlain et al., 2019) often chosen to replicate the average conditions the materials would be subjected to in the joint of interest, these therefore do not fully reflect the range of conditions experience *in vivo*. During a gait cycle, the contact pressure, contact area and cross-shear ratio at the implant surface constantly changes. Computational modelling of a moderately conforming total knee replacement under different kinematic conditions has shown contact pressures ranging from approximately 2.5 to 20 MPa (Abdelgaied et al., 2018); and for a non-optimally aligned implant, edge loading leading to even higher stresses may occur (D' et al., 2001; Cheng et al., 2003; Shiramizu et al., 2009).

The aim of this study was to assess the wear of UHMWPE-on-PEEK-OPTIMA™ under a range of contact pressure and cross-shear conditions. It was hypothesised that due to the similarity in wear performance of PEEK-on-UHMPWE and cobalt chrome-on-UHMWPE in previous knee simulation studies (Cowie et al., 2016a), that the behaviour of the UHMWPE-on-PEEK bearing couple would follow similar trends shown in previous investigations of UHMWPE-on-cobalt chrome under different contact pressure and cross-shear ratio conditions. The research questions asked were:

1. What is the influence of contact pressure on the wear of the UHMWPE-on-PEEK bearing couple?
2. What is the influence of cross-shear ratio on the wear of the UHMWPE-on-PEEK bearing couple?

2. Materials

The pins used were GUR 1020 UHMWPE (non-sterile), consistent with previous studies (Cowie et al., 2016b, 2019), with a truncated cone geometry and a flat contact face ranging from 2 to 7 mm in diameter. The articulating surface of the pins was as machined, consistent with previous pin-on-plate investigations carried out in Leeds (Cowie et al., 2019, 2020; Abdelgaied et al., 2011, 2013, 2018) with an Ra of ~0.1 μm. The PEEK-OPTIMA™ polymer plates (Invibio Ltd., Thornton Cleveleys, UK) were injection moulded with an initial mean surface roughness (Ra) < 0.02 μm, similar to that of previous UHMWPE-on-PEEK pin-on-plate (Cowie et al., 2019, 2020) and knee wear simulation studies (Cowie et al., 2016a, 2023).

3. Methods

The study was carried out using a 6 station multi-axial pin-on-plate reciprocating rig as previously described by Kang et al. (2008a) (Fig. 1). During the test, the plate was fixed into a lubricant containing bath. As the bath reciprocated, the pin rotated via a rack and pinion gear mechanism. The pin and plate motions were in phase, having a common frequency of 1Hz. Throughout the test, a constant axial load was applied to the pin through a mass carrying cantilever mechanism. The lubricant used was 25 % bovine serum (protein concentration ~16 g/l) supplemented with 0.03 % sodium azide solution (v/v) to retard bacterial growth. All tests were carried out under rig running temperature conditions (i.e. no direct heating of the lubricant or environment, ~25 °C)

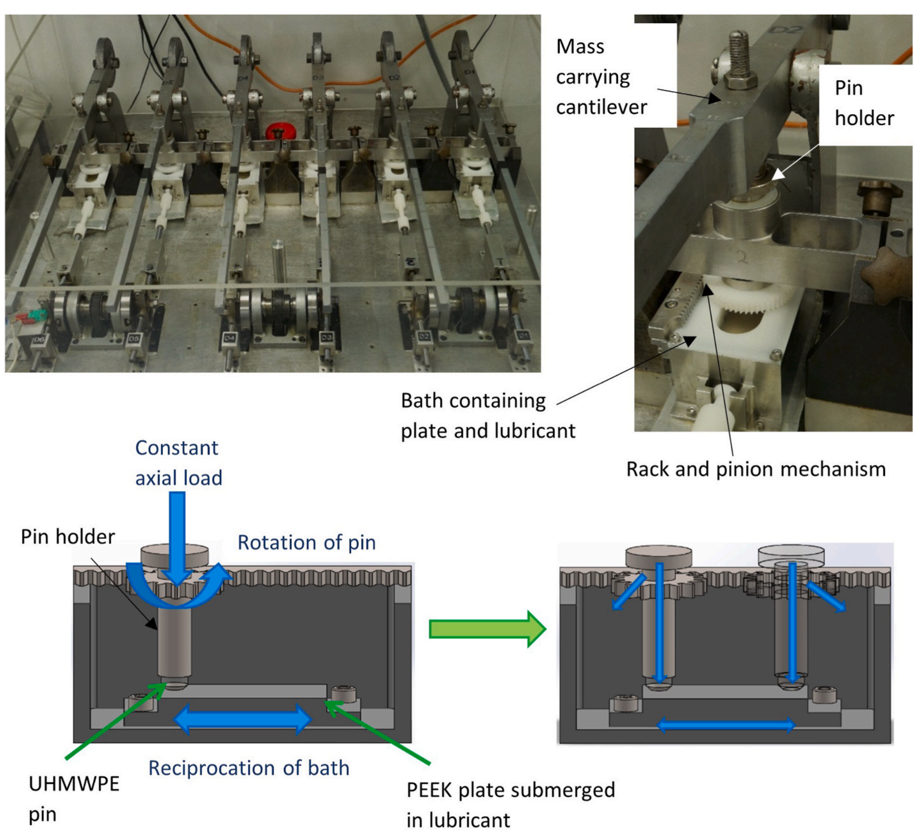

Fig. 1. Top left: photograph of a 6-station pin-on-plate rig with detailed view of the loading beam, bath containing the plate and lubricant, pin holder and rack and pinion mechanism (right). Bottom: a cross section schematic of one station in the pin-on-plate rig, the applied loads and motions are shown by blue arrows.

to minimise test artefacts such as protein precipitation and deposition as previously described by Cowie et al., 2019, 2023.

Prior to the start of the study, the UHMWPE pins were soaked in sterile water for a minimum of 2 weeks to maximise their moisture uptake. The pins were then cleaned ultrasonically in 70% propan-2-ol before being left to stabilise in a temperature and humidity controlled environment. Gravimetric measurements were carried out on an XP26 digital microbalance (Mettler Toledo, Leicester, UK.) with a resolution of 1 μg. Measurements were taken until 5 consecutive measurements fell within a range of ±5 μg with 2 unloaded soak controls used to compensate for uptake of moisture by the polymers. The loss in mass of the pins was converted to a wear volume using a density of 0.934 g/cm^3 for UHMWPE. The wear volume was converted to a wear factor, k, using the following equation (Galvin et al., 2006):

$$k = \frac{V}{PS}$$

Where k is the wear factor (mm^3/Nm), V is the volumetric wear (mm^3), P is the applied load (N) and S the sliding distance (m). The pins were weighed before the start of the study to set a datum then every 0.3 million cycles over the duration of the 0.6 million cycles study. 0.6 million cycles was considered appropriate duration for the wear simulation as previous pin on plate wear simulation of this bearing couple has shown a linear rate of wear over the duration of 1 million cycles wear simulation (Cowie et al., 2019), the shorter duration is consistent with a previous study of UHMWPE-on-metal by Abdelgaied et al. (2018).

Gravimetric analysis of the PEEK plates was carried out however, despite extensive soaking, in excess of 90 days, the data was unreliable and has not been reported. This was likely due to a combination of the low wear of the components and inconsistent moisture uptake of the PEEK.

After the first 24 h of wear simulation, the bulk lubricant temperature was measured daily using a calibrated Fluke 51 II thermocouple (Fluke, Everett, USA) with a resolution of 0.1 °C and an accuracy of ±(0.05% + 0.3 °C). To minimise measurement variability, due to changes in the ambient temperature, the bulk lubricant temperature was expressed as a change from the soak control.

The study matrix, shown in Table 1 was adapted from previous studies by Abdelgaied et al. (2018).

3.1. *Research question 1: influence of contact pressure on the wear of the UHMWPE-on-PEEK bearing couple*

To investigate the influence of contact pressure on the wear of UHMWPE-on-PEEK, the cross-shear ratio was maintained at 0.087 and the contact pressure adjusted by changing a combination of the contact face of the UHMWPE pin and the applied axial load (Table 1). The conditions investigated ranged from 2 to 80 MPa, this represented contact pressures within a range expected for moderately conforming well-positioned knee replacements under activities of daily living (approximately 2.5–30 MPa) (Fregly et al., 2003) and higher contact pressures which may be more representative of a non-conforming or non-optimally-aligned knee replacement (D' et al., 2001; Cheng et al., 2003; Fregly et al., 2003). Between 2.1 and 25.5 MPa, the contact pressure was adjusted by maintaining the load applied to the pin at 80 N and changing the size of the contact face of the pin; above 25.5 MPa, the applied load was increased (Table 1) in line with previous studies by Abdelgaied et al. (2018).

Table 1
Study matrix to investigate the influence of contact pressure and cross-shear ratio on the wear of UHMWPE-on-PEEK.

Study number	Contact area (mm^2)	Applied load (N)	Contact pressure (MPa)	Stroke length (mm)/ rotation (°)	Cross-shear ratio	Sample size
Research question 1: Influence of contact pressure on the wear of UHMWPE						
1	38.5	80	2.1	28/±30	0.087	6
2	19.6	80	4.1	28/±30	0.087	6
3	12.6	80	6.4	28/±30	0.087	5
4	7.1	80	11.3	28/±30	0.087	5
5	3.1	80	25.5	28/±30	0.087	6
6	7.1	212	30	28/±30	0.087	6
7	7.1	283	40	28/±30	0.087	6
8	3.1	252	80	28/±30	0.087	6
Research question 2: Influence of cross-shear ratio on the wear of UHMWPE						
9	12.6	80	6.4	20/0	0	6
10	12.6	80	6.4	10/±10	0.01	6
11	12.6	80	6.4	12/±15	0.022	6
12	12.6	80	6.4	26/±45	0.18	6

3.2. *Research question 2: influence of cross-shear ratio on the wear of the UHMWPE-on-PEEK bearing couple*

To study the influence of cross-shear ratio on UHMWPE wear, the contact pressure was maintained at 6.4 MPa and the cross-shear ratio was varied from 0 (uniaxial motion) to 0.18. The cross-shear ratio was adjusted by altering the stroke length and the size of the pinion. The cross-shear value was determined computationally as previously described by Kang et al. (2008a) and consistent with previous studies carried out on this apparatus (Kang et al., 2008a; Abdelgaied et al., 2013; Galvin et al., 2006). The cross-shear ratios investigated are representative of those occurring during typical motion of total hip and knee joints *in vivo* (Abdelgaied et al., 2011, 2018; Kang et al., 2008a).

A minimum of 5 pin-on-plate bearing combinations (i.e. independent samples) were carried out for each test condition. The mean wear factor for each condition was calculated with 95% confidence limits. Statistical analysis was carried out in SPSS using ANOVA with a post hoc Tukeys test to compare the wear factors in each research question with significance taken at $p<0.05$.

All data are openly available through the University of Leeds Data Repository (Cowie and Jennings, 2023).

4. Results results

4.1. *Research question 1: influence of contact pressure on wear of the UHMWPE-on-PEEK bearing couple*

The mean wear factors with 95% confidence limits of the UHMWPE pins articulating against PEEK plates under a range of contact pressures with a constant cross-shear ratio of 0.087 are shown in Fig. 2. There was a trend of decreasing mean wear factor with increasing contact pressure ($p<0.001$). Between 2.1 and 25.5 MPa, where the contact pressure was

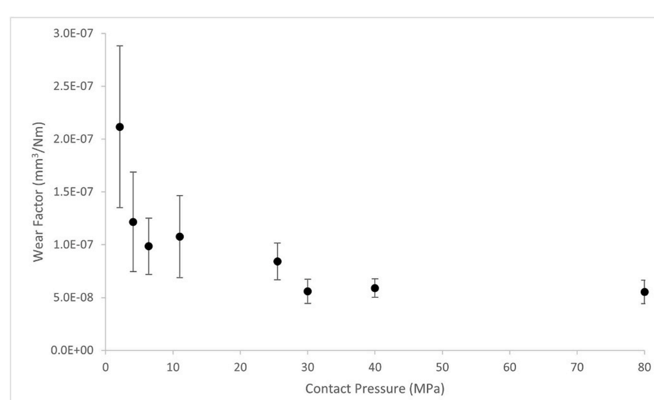

Fig. 2. Mean wear factor (mm^3/Nm) ± 95% confidence limits of UHMWPE pins articulating against PEEK-OPTIMA™ plates under contact pressures from 2.1 to 80 MPa, minimum 5 samples per condition.

adjusted by maintaining the applied load and changing the contact area of the pin, the variability in the wear of UHMWPE was highest when the pin with the largest contact area was used (2.1 MPa); the larger pin contact face also resulted in a higher bulk lubricant temperature (Table 2) although this difference was not significant (p=0.061). The highest bulk lubricant temperatures were recorded for contact pressures > 30 MPa, when the applied loads were highest, and resulting wear factors (and their variability) were at their lowest.

4.2. Research question 2: influence of cross-shear ratio of the UHMWPE-on-PEEK bearing couple

Under uniaxial motion (cross-shear ratio = 0), the wear factor of UHMWPE against PEEK was low (2.96 x 10^{-8} ± 1.36 x10^{-8} mm^3/Nm); introducing multi-directionality to the motion increased the wear factor >3-fold for all the conditions investigated (Fig. 3). One-way ANOVA showed a significant difference ($p<0.01$) in wear factor of the UHMWPE pins under different cross-shear ratio conditions however, post hoc analysis showed only the study carried out under uni-directional motion to be significantly different from the other conditions investigated. There was no significant difference in bulk lubricant temperature (Table 2) between any of the cross-shear ratios investigated, p=0.31, with all differences <1.5 °C.

For all conditions investigated, the wear of the UHMWPE pin was linear over the duration of the study. At the conclusion of the studies, the machining marks in the polyethylene pin had been removed leaving a polished contact face; the PEEK plates also had a polished region and within this, linear scratches were visible. Analysis of the surface topography of the plates using a contacting Form Talysurf (Taylor Hobson, Leicester, UK) with a 2 µm conical tip stylus is available through the University of Leeds Data repository (Cowie and Jennings, 2023). No plastic deformation or structural failure (eg. delamination) of either the UHMWPE or PEEK was observed under any of the conditions investigated.

5. Discussion

The aim of these investigations was to systematically investigate the wear of UHMWPE-on-PEEK under a range of contact pressure and cross-shear conditions representative of the conditions the materials would be subjected to in a total knee replacement. This was achieved using a series of simple geometry pin-on-plate studies.

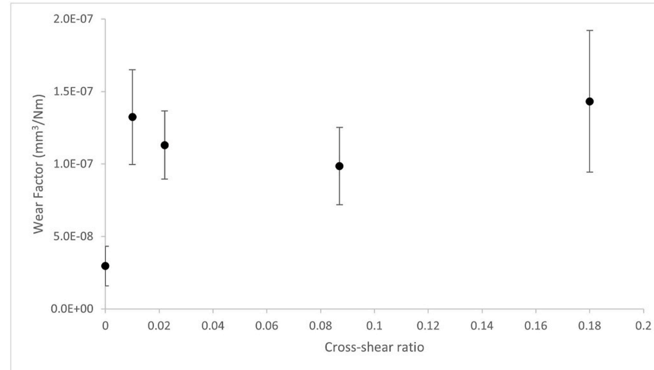

Fig. 3. Mean wear factor (mm^3/Nm) ±95% confidence limits of UHMWPE pins articulating against PEEK-OPTIMA™ plates under contact pressures ranging from 0 to 0.18, n=6.

5.1. Research question 1: influence of contact pressure on wear of the UHMWPE-on-PEEK bearing couple

The studies showed a decrease in wear factor with increasing contact pressure with the rate of change in wear factor greater at the lower contact pressures investigated. These results are consistent with previous investigations of UHMWPE-on-metal carried out in a similar configuration and under similar conditions (Liu et al., 2011; Abdelgaied et al., 2013, 2018; Barbour et al., 1997) and a comparison between the wear factor of UHMWPE-on-PEEK and UHMWPE-on-cobalt chrome (Abdelgaied et al., 2018) is shown in Fig. 4. Archard's law for metallic sliding surfaces states that wear is proportional to applied load and sliding distance (Archard and Hirst, 1956). For polyethylene, wear factor is also dependant on cross-shear and contact pressure (Liu et al., 2011). In this investigation of contact pressure, the sliding distance and the cross-shear were constant throughout the studies. Under low contact pressure conditions, the wear factor of UHMWPE was higher against cobalt chrome than against PEEK polymer; under higher contact pressure conditions, the wear factor of UHMWPE was similar irrespective of the opposing counterface material. Between 2.1 and 25.5 MPa, the contact pressure was changed by altering the diameter of the contact face of the pin, in the UHMWPE-on-PEEK study, there was a larger variability in the wear factor of the larger contact area pins compared to the studies carried out using pins with a smaller contact face. In studies of UHMWPE-on-cobalt chrome carried out under similar conditions, this

Table 2
Mean increase in bulk lubricant temperature ± 95% confidence limits compared to soak control (°C) for each condition investigated, minimum 5 samples per condition.

Study number	Contact area (mm^2)	Contact pressure (MPa)	Cross-shear ratio	Increase in bulk lubricant temperature compared to soak control (°C)
Research question 1: Influence of contact pressure on the wear of UHMWPE				
1	38.5	2.1	0.087	1.7 ± 1.0
2	19.6	4.1	0.087	1.5 ± 0.9
3	12.6	6.4	0.087	1.4 ± 1.0
4	7.1	11.3	0.087	1.3 ± 1.0
5	3.1	25.5	0.087	1.0 ± 0.6
6	7.1	30	0.087	1.8 ± 0.1
7	7.1	40	0.087	2.2 ± 0.4
8	3.1	80	0.087	2.0 ± 0.3
Research question 2: Influence of cross-shear ratio on the wear of UHMWPE				
9	12.6	6.4	0	1.0 ± 0.7
10	12.6	6.4	0.01	0.7 ± 0.6
11	12.6	6.4	0.022	0.9 ± 0.7
12	12.6	6.4	0.18	1.5 ± 0.8

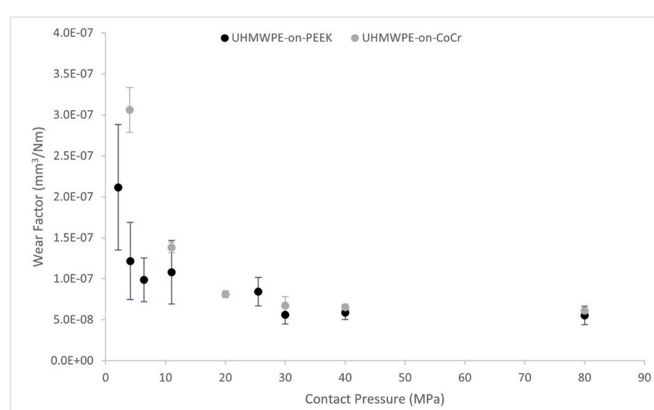

Fig. 4. Mean wear factor ± 95% confidence limits of UHMWPE pins articulating against PEEK-OPTIMA™ plates under contact pressures from 2.1 to 80 MPa, minimum n=5. Data compared to the mean wear factor ± 95% confidence limits of moderately cross-linked UHMWPE-on-CoCr (cobalt chrome) of similar initial surface topography from Abdelgaied et al. (Abdelgaied et al., 2018).

finding was less apparent (Abdelgaied et al., 2013, 2018). Previous investigations of the UHMWPE-on-PEEK bearing couple in both simple geometry (Baykal et al., 2016; Cowie et al., 2020; Heuberger et al., 2021) and whole joint simulation (Cowie et al., 2023) have also shown a higher variability for the UHMWPE-on-PEEK bearing couple compared to UHMWPE-on-CoCr. This is likely not as a result of the experimental set up as in the majority of these studies, the different bearing couples have been tested side-by-side. The materials and possibly the scratching on the surface of the PEEK may have influenced the variability.

5.2. Research question 2: influence of cross-shear ratio on wear of the UHMWPE-on-PEEK bearing couple

Cross-shear ratio is a description of the multidirectionality of the relative motion of the pin and plate. A comparison between the wear factor of UHMWPE against PEEK polymer and cobalt chrome counterfaces of similar initial surface topography under different cross shear ratio conditions is shown in Fig. 5. Against both materials, when articulated with uniaxial motion (cross shear ratio = 0), the wear of UHMWPE was low, introducing multidirectionality into the motion led to an increase in wear factor of UHMWPE. The wear factor of UHMWPE against PEEK was consistently lower than against cobalt chrome under multiaxial conditions. This difference in the magnitude of the wear factor was particularly surprising as in the study by Abdelgaied et al. (2018), a higher contact pressure was used (11 MPa compared to 6.4 MPa in the current study) and a trend of lower wear with increasing contact pressure would be anticipated. For conventional (non cross-linked) polyethylene, under uniaxial motion, polyethylene molecules align with the sliding direction leading to strain hardening of the polyethylene and an improved resistance to wear in that direction. Under multi-axial motion, the polyethylene molecules align with the principal direction of sliding, however, the bonds between the molecular chains are relatively weak. When motion occurs transverse to the principal direction of sliding, orientation softening occurs which accelerates wear (Wang, 2001; Wang et al., 1997). The wear of UHMWPE in the UHMWPE-on-PEEK bearing couple likely follows a similar mechanism of strain hardening and orientation softening similar to that of UHMWPE-on-cobalt chrome. The elevated wear factor of UHMWPE against PEEK under multiaxial compared to uniaxial motion has previously been reported (Heuberger et al., 2021). Increasing cross-shear had no influence on bulk lubricant temperature.

Previous simple geometry tribological studies in which PEEK has been used as a counterface has shown a cross-shear dependency against both cobalt chrome (Brockett et al., 2016) and in a self-mating PEEK

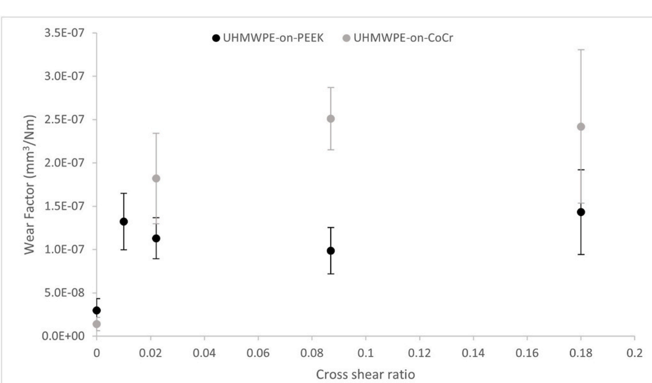

Fig. 5. Mean wear factor ± 95% confidence limits of UHMWPE pins articulating against PEEK-OPTIMA™ plates under cross-shear ratio conditions from 0 to 0.18, contact pressure 6.4 MPa minimum n=5. Data compared to the mean wear factor ± 95% confidence limits of moderately cross-linked UHMWPE-on-CoCr (cobalt chrome) of similar initial surface topography, contact pressure 11 MPa from Abdelgaied et al. (Abdelgaied et al., 2018).

bearing couple (Chamberlain et al., 2019) thought to be driven by similar strain hardening and orientation softening mechanisms as polyethylene. In this study, it was not possible to assess the wear of PEEK gravimetrically (using a balance with readability 0.01 mg) due to inconsistencies in the moisture uptake. Nor was it possible to assess PEEK wear using a geometric technique because although there was a polished region on the plate in which some scratching was observed, there was no defined wear scar. This finding was consistent with previous pin-on-plate wear simulation of the UHMWPE-on-PEEK bearing couple carried out in Leeds (Cowie et al., 2019). Characterisation of the surface topography of the plates post-test showed an increase in surface roughness in the wear scar due to the scratching visible on the plates but with no significant difference ($p>0.05$) in post-test Ra, Rv or Rp between the different test conditions (Cowie and Jennings, 2023). No gross failure or delamination of either PEEK or UHMWPE was observed under any of the conditions investigated (Baykal et al., 2016).

6. Limitations

There were a number of limitations which should be considered when applying the findings from this simple geometry study. Firstly, the test conditions are a simplification of those the materials would be subjected to *in vivo* for example, the pin is under constant load and the simulation is run continuously bringing about the potential for test artefacts. However, pin-on-plate simulation allows the isolation and investigation of individual variables to gain a better understanding of the bearing material combination (Minakawa et al., 1998) and the continuous running of the simulator allows wear simulation to be accelerated. The advantage of pin-on-plate simulation was that a range of contact pressure and cross-shear conditions could be systematically investigated. The studies were of relatively short duration, carried out for 0.6 million cycles, this is consistent with previous work by Abdelgaied et al. (2018) and previous pin-on-plate simulation of this bearing couple over a longer duration (1 million cycles) has shown a linear wear rate (Cowie et al., 2019, 2020). The components used were not sterile or crosslinked. In the proposed total knee replacement (Cowie et al., 2016a), polyethylene will be sterilised by ethylene oxide, which does not induce cross-linking nor influence mechanical or wear properties (Kurtz et al., 2016). However, care should be taken when applying the findings from this study to different polyethylene grades and cross-linking which may behave differently. Finally, it was not possible to assess wear of the PEEK plates, despite extensive soaking (>90 days) and stabilisation of the PEEK (>72 h), assessing wear by gravimetric analysis was unreliable and the change in the geometry of the plates was insufficiently high to assess using geometric techniques. When investigating all-polymer bearing couples where there is potential to lose material from both counterfaces, assessment of the wear of both counterfaces and characterisation of the resulting debris would give a better understanding of the osteolytic potential of the implant (Fisher et al., 2001).

7. Conclusion

For UHMWPE articulating against PEEK OPTIMA™ in a simple geometrical configuration, there was a trend of decreasing UHMWPE wear factor with increasing contact pressure. Under uniaxial motion (cross-shear ratio = 0), the wear of UHMWPE was low, introducing multi-axial motion increased the wear of the UHMWPE. With varying contact pressure and cross-shear ratio, the wear of UHMWPE against PEEK OPTIMA™ polymer showed similar trends to previous studies of UHMWPE-on-cobalt chrome.

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CRediT authorship contribution statement

Raelene M. Cowie: Writing – original draft, Methodology, Investigation, Formal analysis, Data curation, Conceptualization. **Adam Briscoe:** Writing – review & editing, Resources, Conceptualization. **Louise M. Jennings:** Writing – review & editing, Supervision, Resources, Project administration, Methodology, Funding acquisition, Formal analysis, Conceptualization.

Declaration of competing interest

AB is a paid employee of Invibio Ltd., LMJ is a consultant to Invibio Ltd.

Data availability

The data associated with this paper are openly available from the University of Leeds Data Repository. https://doi.org/10.5518/1419. Additional supplementary data has been included with the manuscript.

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Appendix A. Supplementary data

Supplementary data related to this article can be found at https://doi.org/10.1016/j.jmbbm.2023.106196.

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