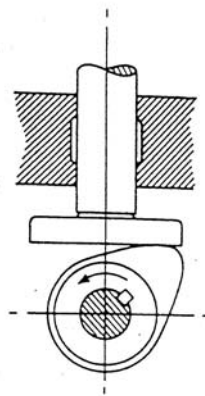


Study on Elastohydrodynamic Lubrication Motion Using Optical Interferometry and Inverse Approach

報告人: 朱力民

研究動機---Gear, Cam, Ball bearing



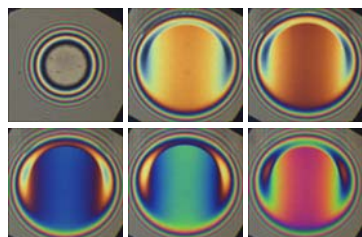
Line contact

Point contact

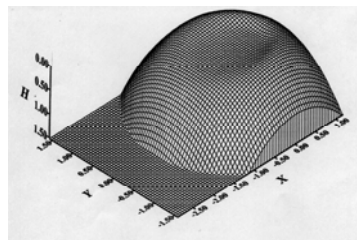


研究動機---逆解法

光學干涉法



影像處理



壓力分佈
黏度分佈

希望發展一套快速且準確的逆解法且可自動修正誤差值，只需使用少數的量測點即可得到準確的黏度值。並且結合實驗與實驗值比較，以驗證本文所提出方法的準確性。



理論分析(MLMI-複層網格法及複層積分法)

1. Reynolds equation :

$$\frac{\partial}{\partial X} \left\{ \frac{\bar{\rho} H^3}{\bar{\eta}_f} \frac{\partial P}{\partial X} \right\} + \frac{\partial}{\partial Y} \left\{ \frac{\bar{\rho} H^3}{\bar{\eta}_f} \frac{\partial P}{\partial Y} \right\} = \lambda \frac{\partial}{\partial X} \{ \bar{\rho} H \}, \quad \lambda = \frac{12 \eta_0 \bar{u} R_x^2}{b^3 p_h}$$

2. Film thickness equation (elastic deformation) :

$$H = H_{00} + \frac{X^2 + Y^2}{2} + \frac{2}{\pi^2} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{P(X', Y') dX' dY'}{[(X - X')^2 + (Y - Y')^2]^{1/2}}$$

3. Force balance equation :

$$\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} P(X, Y) dX dY = \frac{2\pi}{3}$$

4. The density-pressure relationship equation:

$$\rho = \rho_0 \left(1 + \frac{0.6 \times 10^{-9} p}{1 + 1.7 \times 10^{-9} p} \right)$$

5. The viscosity-pressure relationship equation:

$$\eta = \eta_0 \exp \{ (9.67 + \ln \eta_0) [-1 + (1 + 5.1 \times 10^{-9} p)^2] \}$$

Boundary conditions :

$$P = 0, \quad X = X_{in}; \quad -1.8 \leq Y \leq 1.8$$

$$P = 0, \quad Y = \pm 1.8; \quad X_{in} \leq X \leq X_{end} = \zeta(Y)$$

$$P = \frac{dP}{dX} = 0, \quad X = \zeta(Y), \quad -1.8 \leq Y \leq 1.8$$

理論分析(以逆解法求壓力)

在定負荷狀態下，將油膜厚度方程式及負荷平衡方程式以矩陣表示：

$$\mathbf{H}=\mathbf{D}\mathbf{P}\text{----(Direct Inverse)} \quad (2-1) \text{DI}$$

可將待求的壓力分佈值表示為一適當函數，因此可將 \mathbf{P} 矩陣表示為：

$$\mathbf{P}=\mathbf{F}\mathbf{A} \quad (2-5)$$

將(2-5)式代入(2-1)式中可寫為：

$$\mathbf{H}=\mathbf{D}\mathbf{F}\mathbf{A} \quad (2-6) \text{FA}$$

實際的油膜厚度量測值與估測的油膜厚度值是有差異的，比較量測值

$\mathbf{H}^{\text{measured}}$ 與估測值 $\mathbf{H}^{\text{estimated}}$ 間之差異，其誤差函數表為：

$$g = (\mathbf{H}^{\text{estimated}} - \mathbf{H}^{\text{measured}})^T (\mathbf{H}^{\text{estimated}} - \mathbf{H}^{\text{measured}}) \quad (2-7)$$

將 g 對 \mathbf{A} 作一次微分，可得極小值之狀態。

$$\frac{\partial g}{\partial \mathbf{A}} = 0 \quad (2-8)$$

即可得：

$$\mathbf{A} = [(\mathbf{D}\mathbf{F})^T (\mathbf{D}\mathbf{F})]^{-1} (\mathbf{D}\mathbf{F})^T \mathbf{H} \quad (2-9)$$

5

理論分析(潤滑油黏度的計算) I.A.

潤滑劑密度與壓力的關係式(Dowson 和 Higginson)：

$$\bar{\rho} = \frac{\rho}{\rho_0} = 1 + \frac{0.6 \times 10^{-9} p}{1 + 1.7 \times 10^{-9} p} \quad (2-2)$$

潤滑劑黏度與壓力的關係式(Roelands)：

$$\bar{\eta} = \exp \{ (9.67 + \ln \eta_0) [-1 + (1 + 5.1 \times 10^{-9} p)^z] \} \quad (2-3)$$

將 P 、 H 代入雷諾方程式中加以整理可寫成下式：

$$\frac{\partial \bar{\eta}}{\partial P} = c_1 \bar{\eta} + c_2 \bar{\eta}^2 \quad \text{、} \quad (\xi = \partial \bar{\eta} / \partial P - c_1 \bar{\eta} - c_2 \bar{\eta}^2) \quad (2-4)$$

最小均方根誤差法採用下列式子可達到最小化：

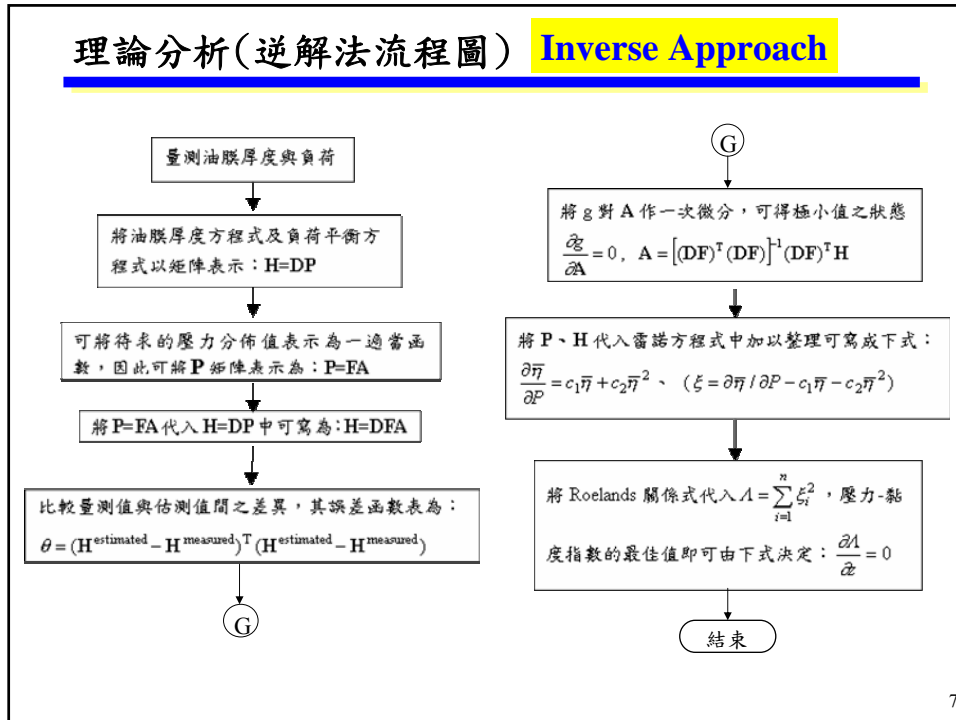
$$A = \sum_{i=1}^n \xi_i^2 \quad (2-10)$$

將(2-3)式代入(2-10)式，Roelands關係式的壓力-黏度指數的最佳值即可由下式決定：

$$\frac{\partial A}{\partial z} = 0 \quad \text{Inverse Approach} \quad (2-11)$$

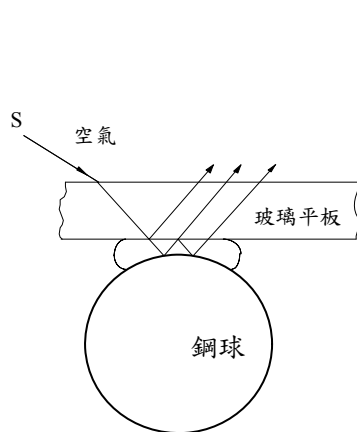
6

理論分析(逆解法流程圖) Inverse Approach



7

Gohar和Cameron

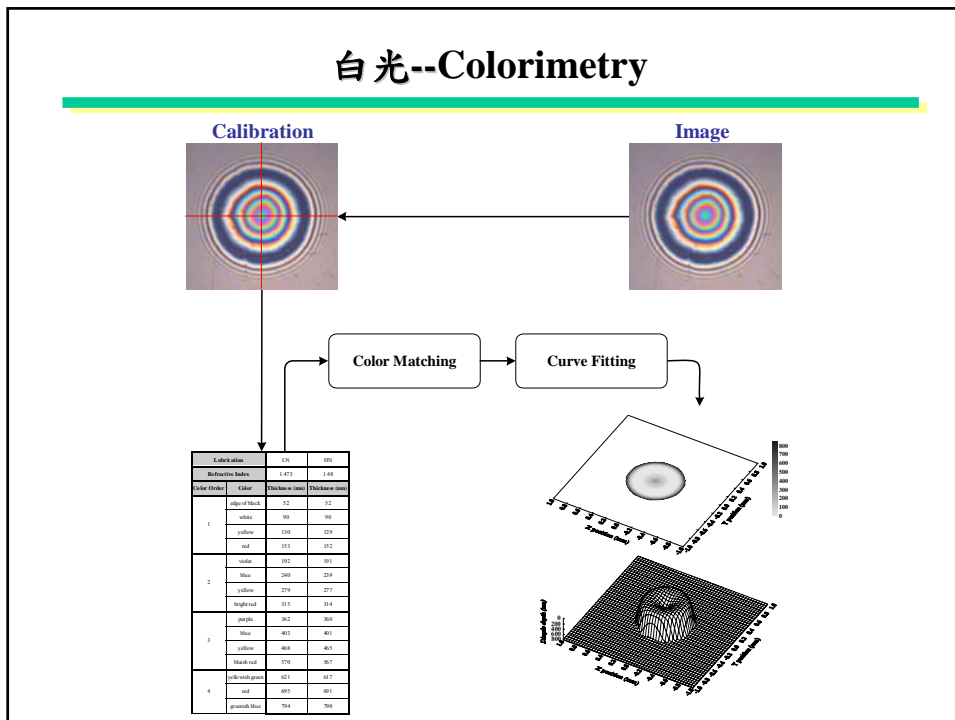


油膜厚度的量測，光學干涉法成為最廣泛的使用技術。

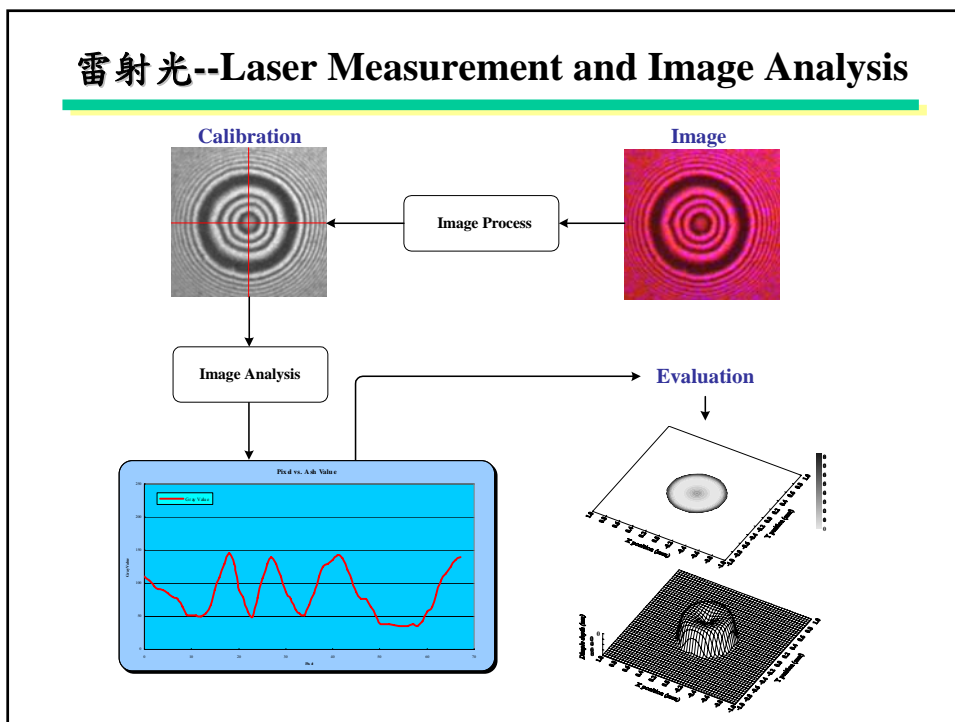
白光 雷射光

潤滑油種類 顏色等級	LN (n=1.473)	
	顏色	厚度 (μm)
1	黑色邊緣	0.052
	灰	0.071
	白	0.090
	淡黃	0.116
	黃	0.130
	橘	0.137
	紅	0.153
2	紫	0.192
	靛	0.216
	藍	0.240
	綠	0.269
	黃	0.279
	橘	0.297
	紅	0.315
3	鮮紅	0.325
	紫	0.362
	靛	0.380
	藍	0.403
	綠	0.432
	黃	0.468
	紅	0.498
4	暗紅	0.570
	暗綠	0.585
	綠	0.610
	黃綠	0.621
	紅	0.695
	綠藍	0.794

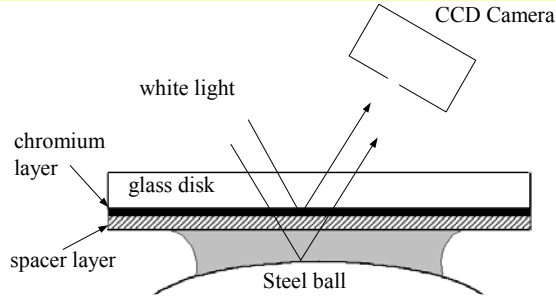
白光--Colorimetry



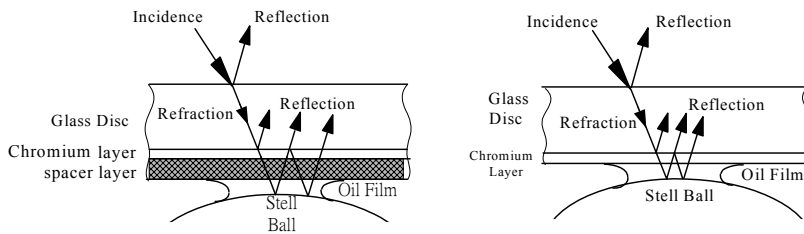
雷射光--Laser Measurement and Image Analysis



Johnston (二氧化矽間隔層)



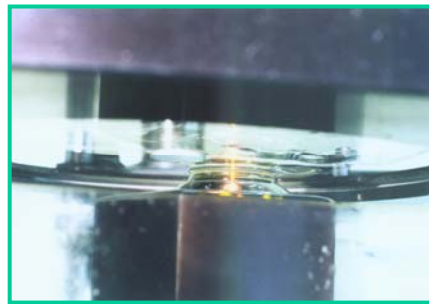
可量測到約15nm的油膜厚度



實驗設備與方法(白光)



光學彈液動潤滑試驗機



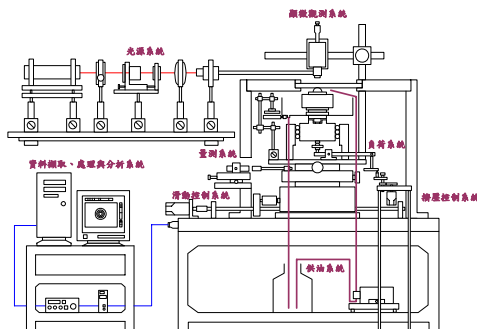
鋼球與光學玻璃圓盤接觸實體圖

實驗設備與方法(雷射光)



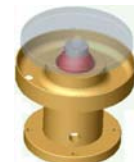
光學彈液動潤滑試驗機(雷射光)

He-Ne雷射光源系統

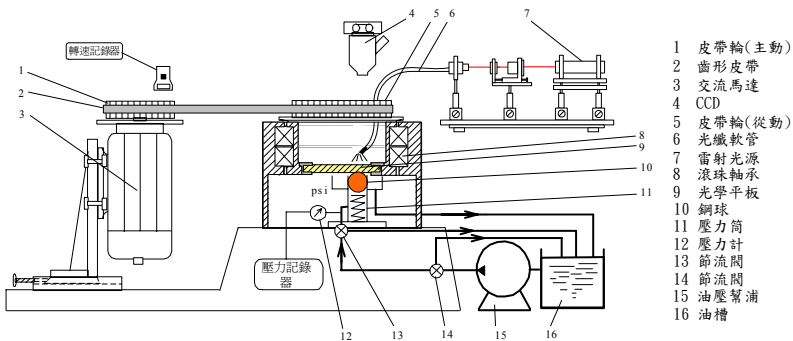


光學彈液動潤滑試驗機示意圖

實驗設備與方法(雷射光)



純滾動情況

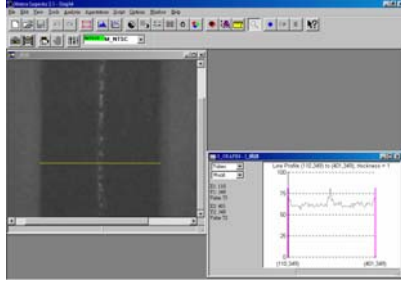


光學彈液動潤滑試驗機示意圖

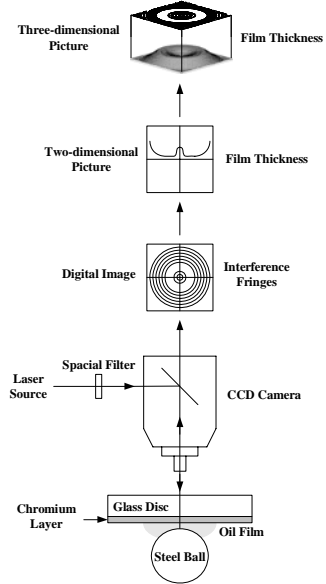
光學觀測系統

油膜分析流程示意圖

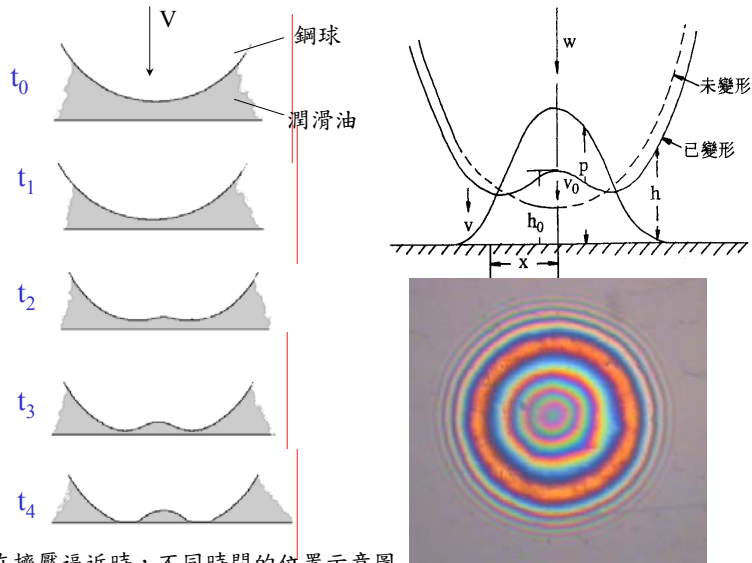
解析度校正圖



鋼線直徑(mm)	所佔的畫素(pixel)	解析度(mm/pixel)
0.602	291	$\frac{0.602}{291} = 2.069 \times 10^{-3}$



EHL of circular contacts at squeeze motion

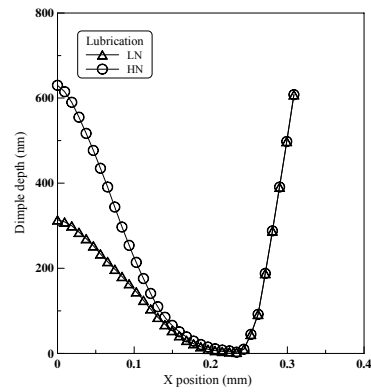
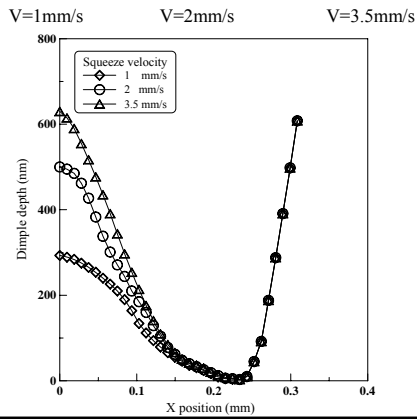
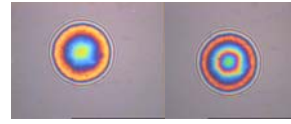
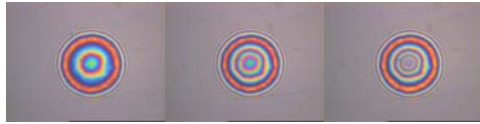


鋼球在擠壓逼近時，不同時間的位置示意圖

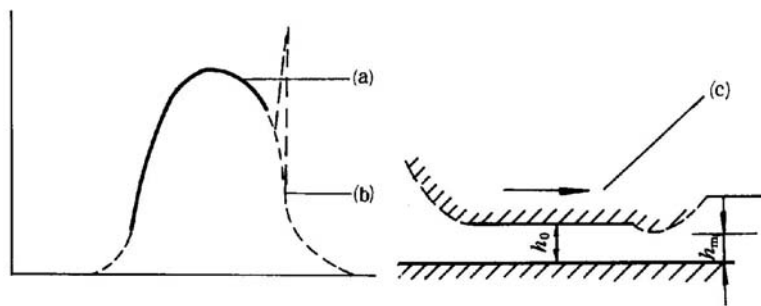
純擠壓狀態下之彈液動潤滑油膜厚度(速度效應、黏度)

潤滑油為HN，負荷為26.58N

擠壓速度為1mm/s



彈液動潤滑油膜形狀與壓力分佈

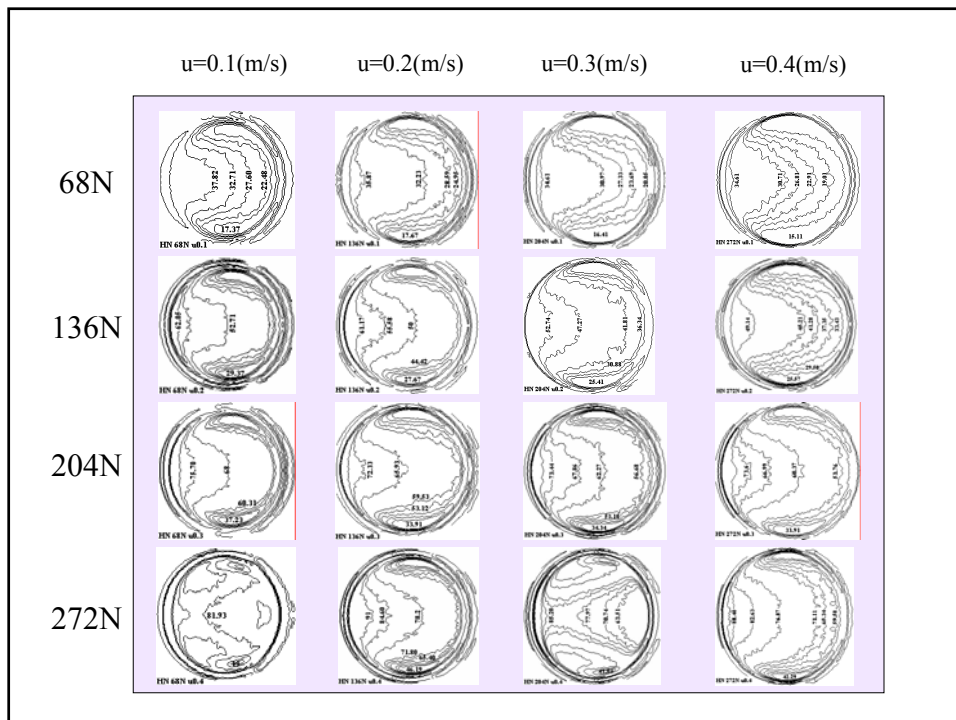
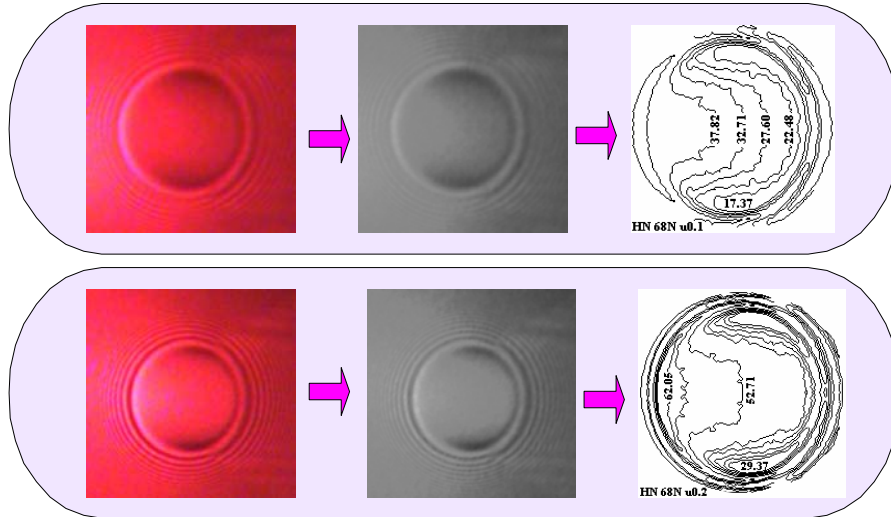


(a) 赫茲壓力分佈

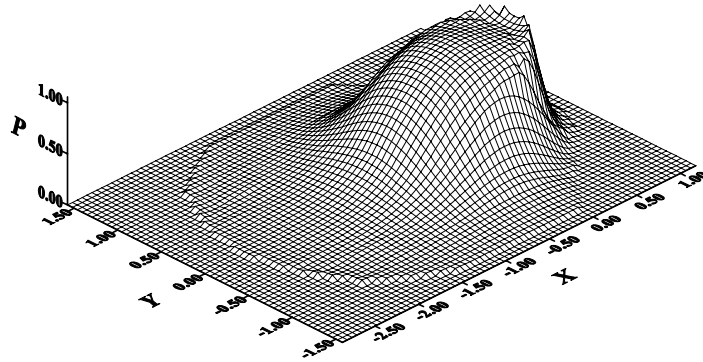
(b) 彈性液體動壓分佈

(c) 物體表面彈性液體動壓潤滑變形

繪製2D油膜等高線圖



I.A. in EHL of circular contacts (1)



在 $W = 1.93 \times 10^{-7}$, $U = 1 \times 10^{-11}$, $G = 3500$ 的條件下，油膜量測誤差 $\sigma = 0.01$ 時

使用逆解法(present)求得之壓力立體圖

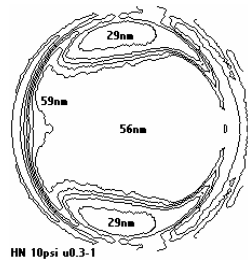
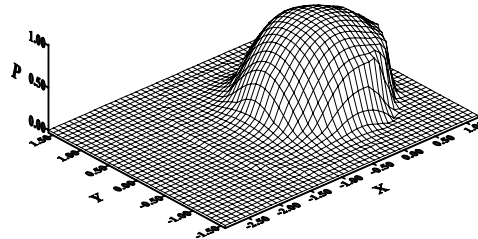
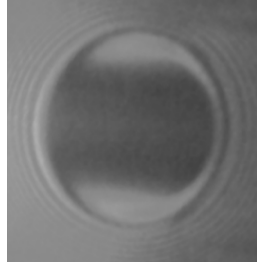
I.A. in EHL of circular contacts (2)

在不同選取範圍、量測誤差、負荷的條件下使用逆解法求得之 z 值

Pressure-viscosity index (Inverse approach)						
Load error X, Y range	$W = 1.0 \times 10^{-6}$			$W = 1.93 \times 10^{-7}$		
	$\sigma=0.0$	$\sigma=0.005$	$\sigma=0.01$	$\sigma=0.0$	$\sigma=0.002$	$\sigma=0.005$
$-1.0 < X < 0.4$ $Y = 0.0$	0.475	0.507	0.512	0.482	0.486	0.498
$\sqrt{X^2 + Y^2} < 0.2$	0.499	0.518	0.523	0.492	0.498	0.515
$\sqrt{X^2 + Y^2} < 0.4$	0.456	0.425	0.431	0.463	0.450	0.435

$\sigma=0.04$ Error= 4.99% , 6nm

I.A. in EHL of circular contacts (3)



HN 10psi u0.3-1

逆解法求出接觸區的壓力分佈值

	z
Actual value	0.8486
Inverse approach	0.9052

Error= 6.67%

灰階干涉條紋圖及油膜分佈輪廓圖

使用逆解法求得之 z 值並與真實值比較

I.A. in EHL of circular contacts at squeeze motion (1)

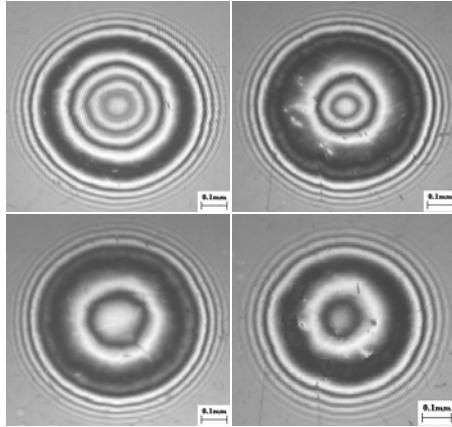
在不同選取範圍、量測誤差、時間點的條件下使用逆解法求得之 z 值

Pressure-viscosity index (Inverse approach)						
t -step	$\Delta t=0.03$ s			$\Delta t=0.06$ s		
X-region	$\sigma=0.0$	$\sigma=0.005$	$\sigma=0.01$	$\sigma=0.0$	$\sigma=0.005$	$\sigma=0.01$
$0.05 < X < 0.9$	0.4882	0.4959	0.5015	0.5037	0.5159	0.5289
$0.05 < X < 0.5$	0.4876	0.4952	0.5002	0.5026	0.5151	0.5272
$0.05 < X < 0.2$	0.4866	0.4946	0.4996	0.5012	0.5147	0.5268

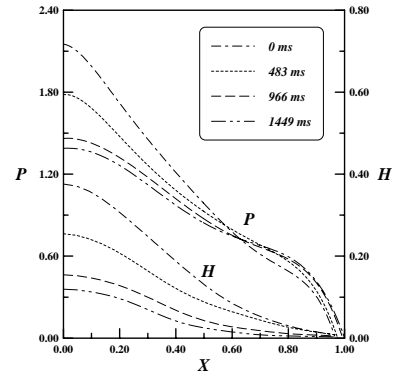
$\sigma=0.04$ Error= 4.77% , 9nm

I.A. in EHL of circular contacts at squeeze motion (2)

擠壓速度為3.5mm/s，負荷為26.58N, HN



四個時間點的灰階干涉條紋圖



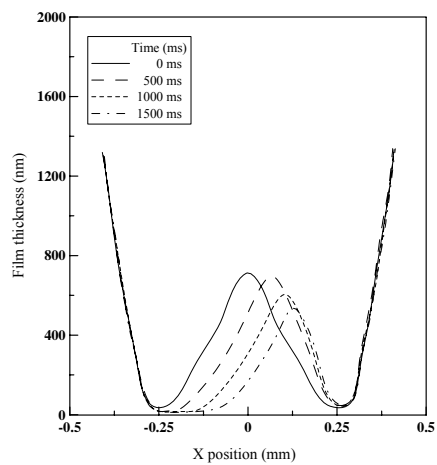
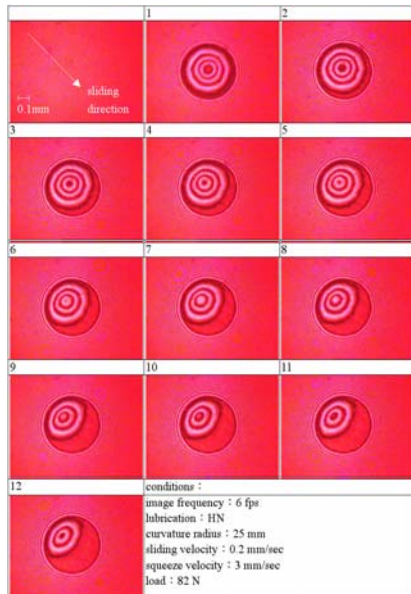
以逆解法求出在四個時間點的壓力分佈值

	z
Actual value	0.8486
Inverse approach	0.8912

Error= 5.02%

使用逆解法求得之 z 值並與真實值比較

Study on the Dynamic Lubrication Characteristics of the Oil Film under the Combined Squeeze and Sliding Motion Using Laser Measurement Method

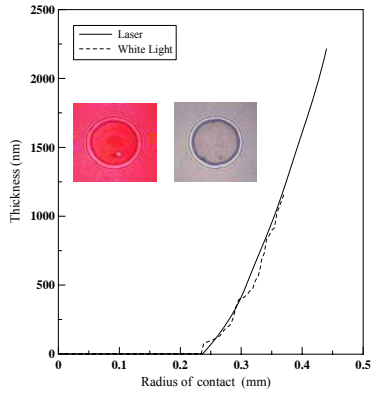


油膜輪廓圖

油膜干涉條紋圖

使用光學干涉法及逆解法研究接觸負荷，彈性模數值

逆解當量彈性模數(E')值



鋼球直徑	實驗負載值(N)	HERTZ接觸直徑(mm)	當量彈性模數(E')	誤差百分比(%)
50mm	57.633	0.50520	135.022	15.502
50mm	83.844	0.57474	132.489	13.335
50mm	110.555	0.63536	129.309	10.615
50mm	133.751	0.68588	124.356	6.378
50mm	158.001	0.72987	121.913	4.289
50mm	181.197	0.76315	122.305	4.623
		E'平均值(*E+09)	127.411	8.993
E'理論值	1.169E+11			

逆解正向負荷(N)值

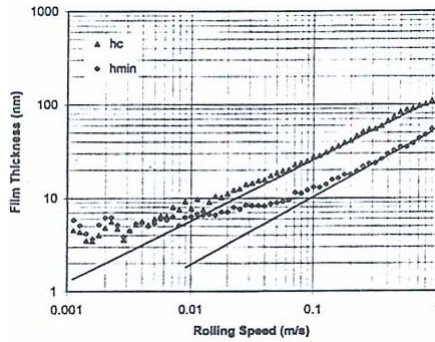
鋼球直徑	HERTZ接觸直徑(mm)	估算負載值(N)	實驗負載值(N)	誤差(%)
50mm	0.50520	50.244	57.633	-12.821
50mm	0.57474	73.979	83.844	-11.766
50mm	0.63536	99.945	110.555	-9.597
50mm	0.68588	125.732	133.751	-5.995
50mm	0.72987	151.504	158.001	-4.112
50mm	0.76315	173.190	181.197	-4.419
			平均負載誤差(%)	-8.118

極薄膜潤滑

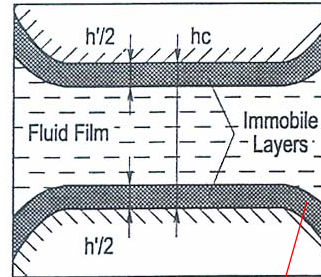
Ultra Thin Film Lubrication

報告人: 朱力民

研究目的---Thin Film Lubrication



Johnston 膜厚值高於彈液動潤滑(EHL)理論的計算值



Hartl, Georges
, Moore 等人

發展出一套彈液動薄膜潤滑理論模式。運用此模式可合理的計算出薄膜潤滑狀態下的油膜厚度值及黏度值

黏度、厚度、壓力分佈值

29

理論分析(TFL- Thin Film Lubrication)

1. Classical EHL

2. EHL Surface Force Model

傳統彈液動潤滑點接觸雷諾方程式如下所示：

$$\frac{\partial}{\partial x} \left\{ \frac{\rho h^3}{\eta} \frac{\partial p_{vis}}{\partial x} \right\} + \frac{\partial}{\partial y} \left\{ \frac{\rho h^3}{\eta} \frac{\partial p_{vis}}{\partial y} \right\} = 12 \frac{\partial}{\partial x} \{ \rho \bar{u} h \} \quad (6-12)$$

凡得瓦力隨膜厚變化的關係式為：[Ref. Jang and Tichy](#)

$$p_{vdw} = -\frac{A}{6\pi h^3}, \quad A \cong 10^{-19} J \quad (6-13)$$

結構力隨膜厚變化的關係式為：

$$P_{solv} = -c \exp(-h/a) \cos(2\pi h/a), \quad a = 1nm, \quad c = 172MPa \quad (6-14)$$

因此在接觸區內薄膜所受的總壓力為：

$$P = P_{vis} + P_{solv} + P_{vdw} \quad (6-15)$$

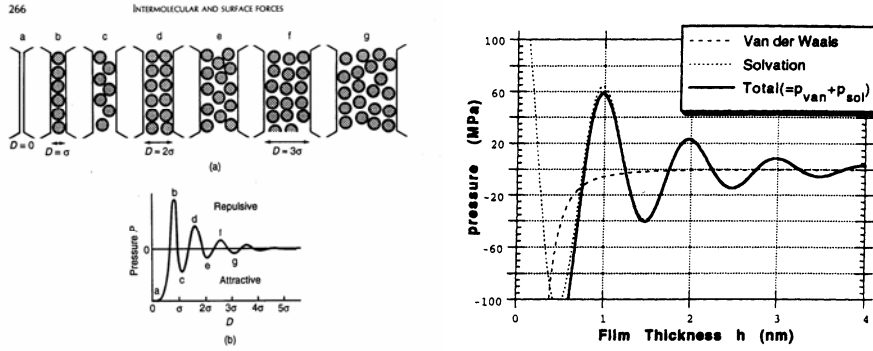
點接觸彈液動薄膜的厚度方程式為：

$$H = H_{00} + \frac{X^2 + Y^2}{2} + \frac{2}{\pi^2} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \frac{P(X', Y') dX' dY'}{[(X - X')^2 + (Y - Y')^2]^{1/2}} \quad (6-9)$$

在點接觸之狀態，垂直負荷容量為：

$$\int_{-\infty}^{\infty} \int_{-\infty}^{\infty} P(X, Y) dX dY = \frac{2\pi}{3} \eta \cdot \rho \quad (6-10)$$

Solvation force



Reference: Jacob N. Israelachvili, Intermolecular and surface forces, (1992).

3. EHTFL (薄膜壓力-黏度指數、吸附層厚度與黏度比值計算)

$$\frac{\partial}{\partial X} \left\{ \frac{\bar{\rho}H^3}{\bar{\eta}_f} \left[1 + \frac{\bar{\delta}}{H} \left(6 - 12 \frac{\bar{\delta}}{H} + 8 \frac{\bar{\delta}^2}{H^2} \right) (\eta^* - 1) \right] \frac{\partial P}{\partial X} \right\} + \frac{\partial}{\partial Y} \left\{ \frac{\bar{\rho}H^3}{\bar{\eta}_f} \left[1 + \frac{\bar{\delta}}{H} \left(6 - 12 \frac{\bar{\delta}}{H} + 8 \frac{\bar{\delta}^2}{H^2} \right) (\eta^* - 1) \right] \frac{\partial P}{\partial Y} \right\}$$

$$= \lambda \frac{\partial}{\partial X} \left\{ \bar{\rho}H \left[1 + \frac{u^*}{u} \left(1 - 2 \frac{\bar{\delta}}{H} \right) \left(\frac{1}{2} - \frac{\bar{\delta}}{\Delta} - \frac{(H - 2\bar{\delta})}{2\Delta\eta^*} \right) \right] \right\} \quad (6-6)$$

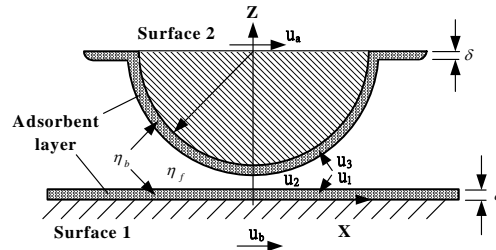
Let:

$$\theta = \left[1 + \frac{\bar{\delta}}{H} \left(6 - 12 \frac{\bar{\delta}}{H} + 8 \frac{\bar{\delta}^2}{H^2} \right) (\eta^* - 1) \right]$$

$$\zeta = \left[1 + \frac{u^*}{u} \left(1 - 2 \frac{\bar{\delta}}{H} \right) \left(\frac{1}{2} - \frac{\bar{\delta}}{\Delta} - \frac{(H - 2\bar{\delta})}{2\Delta\eta^*} \right) \right]$$

$$\varepsilon = \frac{\bar{\rho}H^3}{\bar{\eta}_f}$$

(6-7)



$$\eta^* = \frac{\eta_f}{\eta_b} \quad \bar{\delta} = \frac{\delta R}{b^2} \quad \Delta = \frac{h}{\eta^*} + 2\delta \left(1 - \frac{1}{\eta^*} \right)$$

Velocity Distribution

$$U_1 = \frac{1}{2} A \frac{\eta^*}{\bar{\eta}_f} H^2 \frac{\partial P}{\partial X} Z(Z-1) + U_b$$

$$U_2 = \frac{1}{2} \frac{A}{\bar{\eta}_f} \frac{\partial P}{\partial X} \left[H^2 Z(Z-1) + \eta^* \bar{\delta} (\bar{\delta} - H) \left(1 - \frac{1}{\eta^*}\right) \right] + U_b$$

$$U_3 = \frac{1}{2} A \frac{\eta^*}{\bar{\eta}_f} H^2 \frac{\partial P}{\partial X} Z(Z-1) + U_a$$

$$V_1 = \frac{1}{2} A \frac{\eta^*}{\bar{\eta}_f} H^2 \frac{\partial P}{\partial Y} Z(Z-1)$$

$$V_2 = \frac{1}{2} \frac{A}{\bar{\eta}_f} \frac{\partial P}{\partial Y} \left[H^2 Z(Z-1) + \eta^* \bar{\delta} (\bar{\delta} - H) \left(1 - \frac{1}{\eta^*}\right) \right]$$

$$V_3 = \frac{1}{2} A \frac{\eta^*}{\bar{\eta}_f} H^2 \frac{\partial P}{\partial Y} Z(Z-1) \quad (6-8)$$

Use inverse approach to calculate Z, δ, η^*

$$f = \frac{\partial}{\partial X} \left\{ \varepsilon \theta \frac{\partial P}{\partial X} \right\} + \frac{\partial}{\partial Y} \left\{ \varepsilon \theta \frac{\partial P}{\partial Y} \right\} - \lambda \frac{\partial}{\partial X} \{ \bar{\rho} H \zeta \} \quad (6-16)$$

將其離散化，並將各點誤差平方值累加起來可得：

$$S = \sum_{i=1}^n f_i^2 \quad (6-17)$$

將(6-17)式分別對 z 、 η^* 及 δ 取一次微分可得：

$$\zeta_1 = \frac{\partial S}{\partial z}, \quad \zeta_2 = \frac{\partial S}{\partial \bar{\delta}}, \quad \zeta_3 = \frac{\partial S}{\partial \eta^*} \quad (6-18, 19, 20)$$

為了使上式得到最小值，使用牛頓-瑞佛遜數值法耦合疊代：

$$\begin{aligned} \left(\frac{\partial \zeta_1}{\partial z} \right)^o \Delta z + \left(\frac{\partial \zeta_1}{\partial \bar{\delta}} \right)^o \Delta \bar{\delta} + \left(\frac{\partial \zeta_1}{\partial \eta^*} \right)^o \Delta \eta^* &= -\zeta_1^o \\ \left(\frac{\partial \zeta_2}{\partial z} \right)^o \Delta z + \left(\frac{\partial \zeta_2}{\partial \bar{\delta}} \right)^o \Delta \bar{\delta} + \left(\frac{\partial \zeta_2}{\partial \eta^*} \right)^o \Delta \eta^* &= -\zeta_2^o \\ \left(\frac{\partial \zeta_3}{\partial z} \right)^o \Delta z + \left(\frac{\partial \zeta_3}{\partial \bar{\delta}} \right)^o \Delta \bar{\delta} + \left(\frac{\partial \zeta_3}{\partial \eta^*} \right)^o \Delta \eta^* &= -\zeta_3^o \end{aligned} \quad (6-21)$$

Use inverse approach to calculate Z, δ, η^*

$$\begin{bmatrix} \frac{\partial \zeta_1}{\partial z} & \frac{\partial \zeta_1}{\partial \bar{\delta}} & \frac{\partial \zeta_1}{\partial \eta^*} \\ \frac{\partial \zeta_2}{\partial z} & \frac{\partial \zeta_2}{\partial \bar{\delta}} & \frac{\partial \zeta_2}{\partial \eta^*} \\ \frac{\partial \zeta_3}{\partial z} & \frac{\partial \zeta_3}{\partial \bar{\delta}} & \frac{\partial \zeta_3}{\partial \eta^*} \end{bmatrix}^o \begin{bmatrix} \Delta z \\ \Delta \bar{\delta} \\ \Delta \eta^* \end{bmatrix}^n = - \begin{bmatrix} \zeta_1 \\ \zeta_2 \\ \zeta_3 \end{bmatrix}^o \quad (6-22)$$

使用 Gauss-Seidel 疊代法及 Over-Relaxation 法反覆疊代，以求得壓力-黏度指數值，吸附層厚度與黏度比值。

$$\begin{aligned} z^n &= z^o + R_{f1} \times \Delta z^n \\ \eta^{*n} &= \eta^{*o} + R_{f3} \times \Delta \eta^{*n} \\ \bar{\delta}^n &= \bar{\delta}^o + R_{f2} \times \Delta \bar{\delta}^n \end{aligned} \quad (6-23)$$

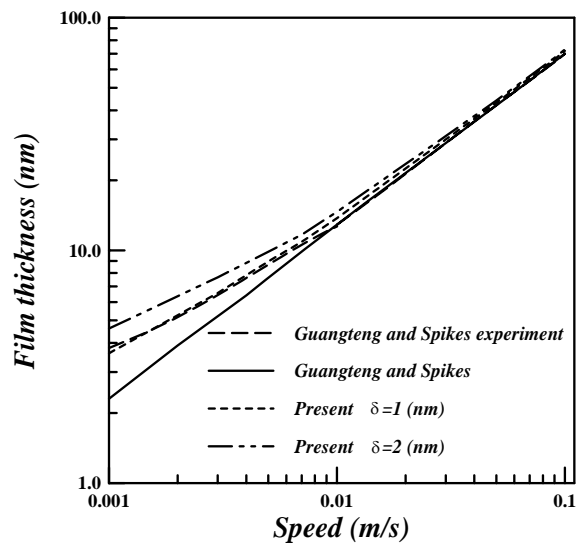
其中：

z^o 、 $\bar{\delta}^o$ 、 η^{*o} ：前一次疊代之值。

z^n 、 $\bar{\delta}^n$ 、 η^{*n} ：此次疊代之值。

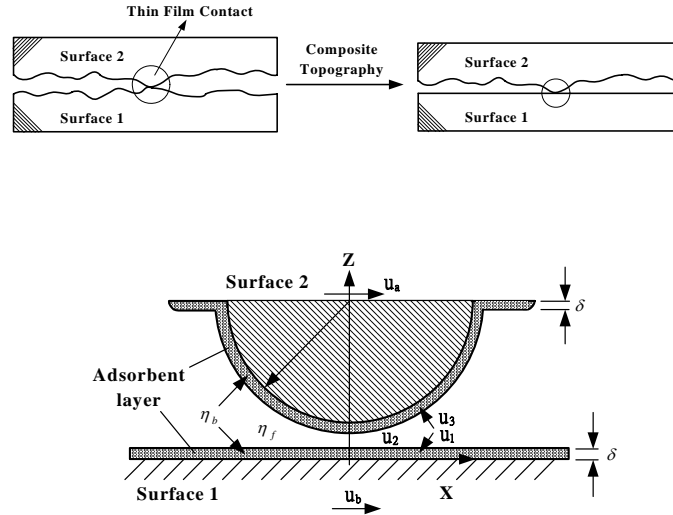
R_{f1} 、 R_{f2} 、 R_{f3} ：鬆弛因子(Relaxation factor)

$\Delta z^n = z^n - z^o$ 、 $\Delta \bar{\delta}^n = \bar{\delta}^n - \bar{\delta}^o$ 、 $\Delta \eta^{*n} = \eta^{*n} - \eta^{*o}$

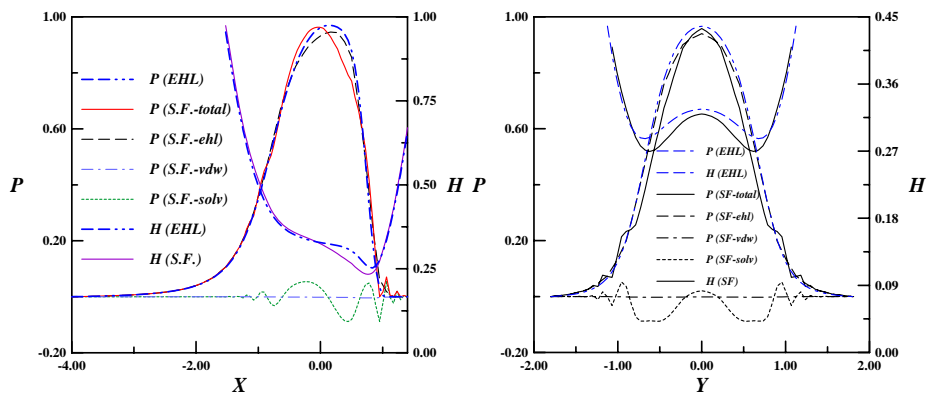


使用彈液動薄膜潤滑模式，吸附層取1及2nm的條件下，計算中心油膜厚度值隨速度變化的關係並與Guangteng和Spike所作的實驗值比較

由承載面間之微凸體接觸所產生點接觸彈液動薄膜潤滑問題



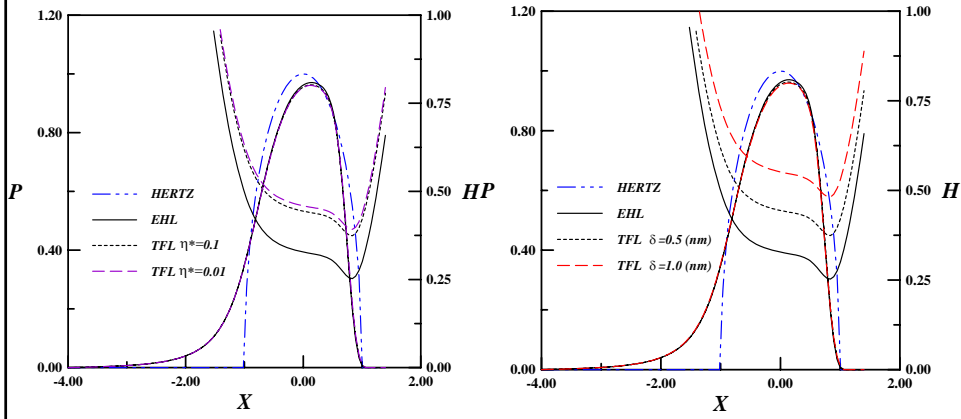
Thin Film Lubrication (1)



表面力模式所計算出在X軸上壓力及油膜厚度分佈值

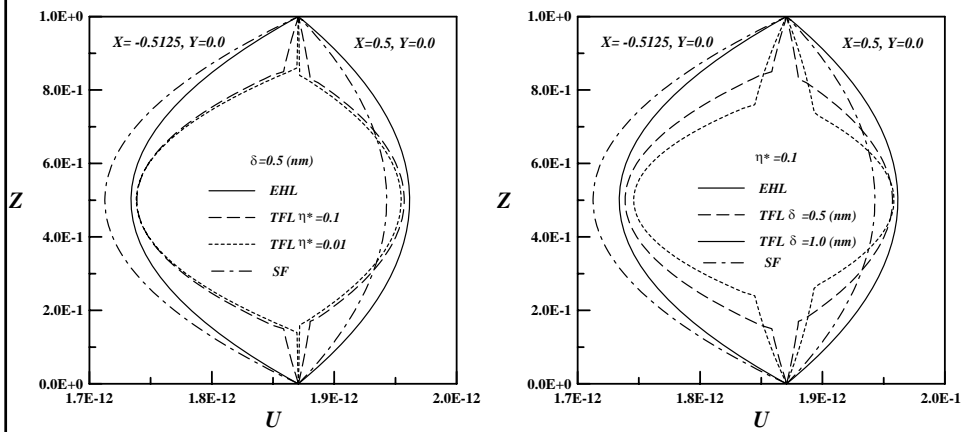
表面力模式所計算出在Y軸上壓力及油膜厚度分佈值

Thin Film Lubrication (2)



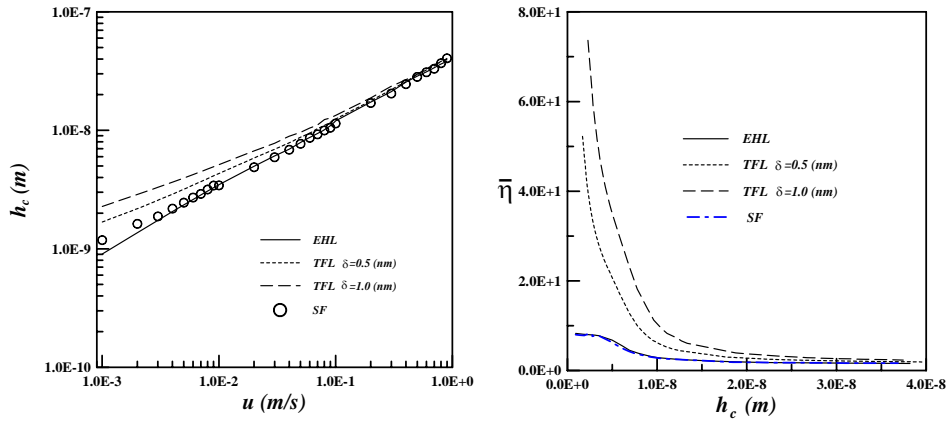
彈液動薄膜潤滑模式在純滾動、定負荷、不同吸附層厚度及不同黏度比條件下，X軸之壓力及油膜厚度分佈值

Thin Film Lubrication (3)



使用彈液動薄膜潤滑模式在純滾動、定負荷、不同吸附層厚度及不同黏度比條件下，不同層中X方向速度分佈值

Thin Film Lubrication (4)

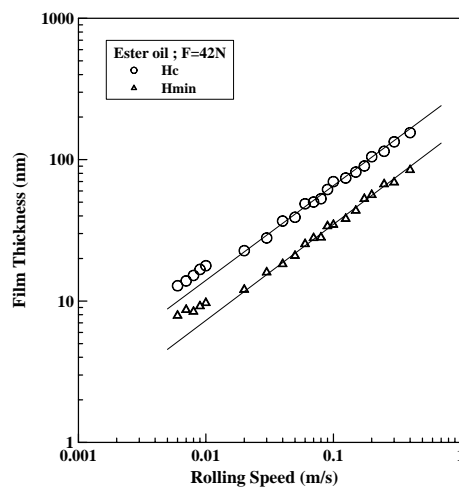


使用彈液動薄膜潤滑與表面力模式求得中心油膜厚度隨著速度變化的關係

使用彈液動薄膜潤滑模式求得油膜中心厚度隨黏度變化的關係

2.27nm, $\delta=0.5$ nm, 5倍,
 $\delta=1.0$ nm, 9倍

Thin Film Lubrication (5)



Ester潤滑油在負荷42N之條件下速度與膜厚的關係

Thin Film Lubrication (6)

使用彈液動潤滑逆解法求得之 z 值並與真實值比較

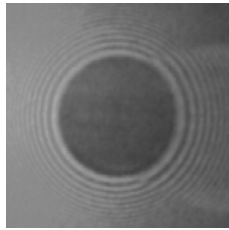
	z
Actual value	0.8195
Inverse approach	0.9093

Error= 10.96%

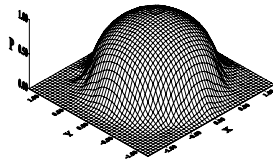
使用彈液動薄膜潤滑逆解法求得之 z 、 η^* 、 δ 值並與真實值比較

	z	η^*	δ (nm)
Actual value	0.8195	0.1429-0.2	0.74-1.45
Inverse approach	0.8629	0.1522	1.1

Error= 5.30%



灰階干涉條紋圖及油膜分佈輪廓圖



逆解法求出接觸區的壓力分佈值

水分子在奈米侷限空間下之行為研究



The study of behaviors of nanoconfined water molecules

報告人: 朱力民

Potentials used in the MD simulation for macromolecules

(Energy Calculation and Dynamics, ENCAD)

$$U_{total} = U_{bond} + U_{bending} + U_{vdw} + U_{coul}$$

U_{bond}	鍵長勢能		<ul style="list-style-type: none"> • 鍵長、鍵角、扭轉角及氫鍵等勢能大多於探討鍵分子結構特性時使用
$U_{bending}$	鍵角勢能		
U_{vdw}	凡得瓦勢能		<ul style="list-style-type: none"> • 庫倫勢能主要是探討電荷間的相互作用力；一般於有機及無機的模擬中都會使用
U_{coul}	庫倫勢能		<ul style="list-style-type: none"> • 分子之間會有一種非常微弱的相互作用力，此種作用力勢能稱之為凡得瓦勢能；一般於有機及無機的模擬中都會使用

Inter-molecular potential

Au-Au

$$E = - \left\{ \sum_j \xi^2 \exp \left[-2q \left(\frac{r_{ij}}{r_0} - 1 \right) \right] \right\}^{1/2} + \sum_j A \exp \left[-p \left(\frac{r_{ij}}{r_0} - 1 \right) \right]$$

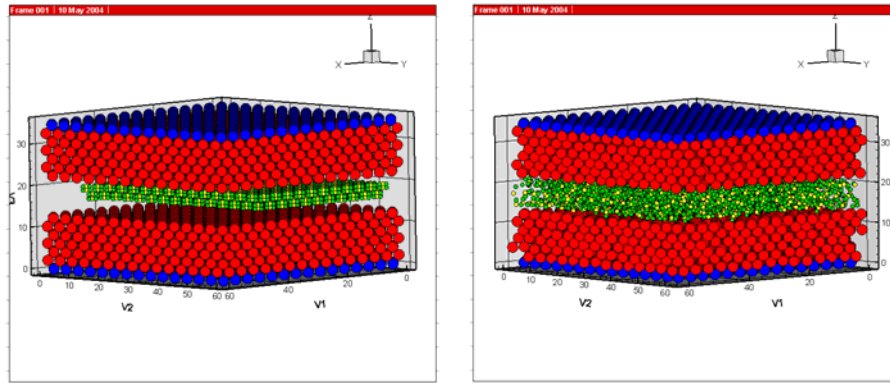
H2O-H2O

$$U = U_{bond} + U_{bend} + U_{vdw} + U_{els}$$

Au-H2O

$$U_{Au-H_2O} = U_{Au-O}(r_{Au-O}) + U_{Au-H1}(r_{Au-H1}) + U_{Au-H2}(r_{Au-H2})$$

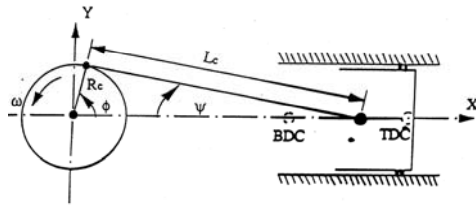
以分子動力學模擬研究水薄膜在不同空間下之現象



Optimum design of piston ring shape using inverse method

Li-Ming Chu^{a*}

活塞-連桿機構配置圖



$$u = R\omega \left(\sin \phi + \frac{R}{2L} \frac{\sin 2\phi}{\sqrt{1 - R^2 \sin^2 \phi / L^2}} \right)$$

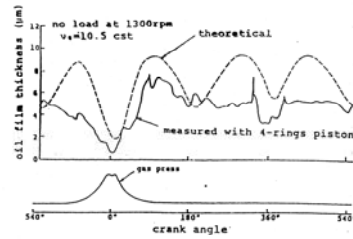
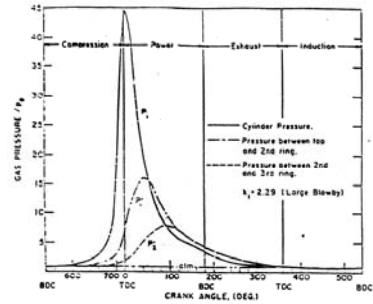


Fig 8 Oil film thickness of a first compression ring/cylinder bore interface

GOVERNING EQUATIONS OF PISTON RING LUBRICATION

The hydrodynamic lubrication, the steady state one-dimensional Reynolds equation is

$$\frac{\partial}{\partial x} \left(\frac{\rho h^3}{\eta} \frac{\partial p}{\partial x} \right) = 6u_b \frac{\partial(\rho h)}{\partial x} \quad (1)$$

where u_b represents the piston velocity. Eq. (1) can be integrated as:

$$\frac{dp}{dx} = 6\eta u_b \frac{h - h_m}{h^3} \quad (2)$$

where h_m is the film thickness at maximum pressure, i.e. $dp/dx = 0$. The dimensionless form of Eq. (2) is

$$\frac{dP}{dX} = 6 \left(\frac{H - H_m}{H^3} \right) \quad (3)$$

The boundary conditions for Eq. (3) are:

$$P = P_b + P_a, \text{ at } X = X_m (=0) \quad (4a)$$

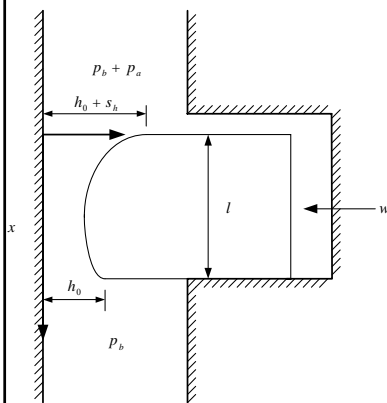
$$P = P_b, \text{ at } X = X_{end} (=1) \quad (4b)$$

The load-carrying capacity of the oil film per unit length is:

$$w = \int_0^1 p dx \quad (5)$$

The pressure acting on the piston ring in the radial direction is assumed to be composed of the pressure at the inner side of the ring and the piston ring elastic pressure. Therefore, the dimensionless load balance equation for the piston ring is given as:

$$W = \int_0^1 P dX = P_s + P_e \quad (6)$$



Optimum design of piston ring shape using inverse method (1)

$$H_k = (X_k - 1) \sum_{j=1}^{m+1} C_j X_k^j - X_k + (H_0 + 1) \quad (7)$$

$$P_k = (X_k - 1) \sum_{i=1}^{n+1} B_i X_k^i - X_k P_a + (P_b + P_a) \quad (8)$$

Substituting Eq. (8) into Eq. (6), the force balance equation becomes

$$W = (P_b + \frac{1}{2} P_a) - \sum_{i=1}^{n+1} \frac{1}{(i+1)(i+2)} B_i \quad (9)$$

Substituting Eqs. (7) and (8) into Eq. (3), the governing equation becomes

$$f_k = \left\{ -P_a + \sum_{i=1}^{n+1} [X_k^{(i-1)}(2X_k - 1) + (i-1)X_k^{(i-2)}(X_k^2 - X_k)] B_i \right\}$$

$$[(X_k - 1) \sum_{j=1}^{m+1} C_j X_k^j - X_k + (H_0 + 1)]^3 - 6 \left\{ [(X_k - 1) \sum_{j=1}^{m+1} C_j X_k^j - X_k + (H_0 + 1)] - H_m \right\} \quad (10)$$

Optimum design of piston ring shape using inverse method (2)

Hence, to obtain the smallest error between the direct and estimated values, the least-square error method and variational method are employed here subject to the force balance constraint. The least-square error method and variational method require the residual function to be minimized.

$$\frac{\partial G}{\partial B_i} = 0, \quad i = 1, 2, 3, \dots, n+1$$

$$\frac{\partial G}{\partial C_j} = 0, \quad j = 1, 2, 3, \dots, m+1$$

where the residual function with Lagrange multiplier λ is

$$G = \sum_{k=1}^n f_k^2 + \lambda [W - (P_b + \frac{1}{2} P_a) + \sum_{i=1}^{n+1} \frac{1}{(i+1)(i+2)} B_i]$$

Eqs. (12) and (13) can be rewritten as:

$$\sum_{k=1}^n \beta_{ik} \alpha_k + \frac{0.5}{(i+1)(i+2)} \lambda = \sum_{k=1}^n \beta_{ik} \xi_k, \quad i = 1, 2, 3, \dots, n+1$$

$$\sum_{k=1}^n \gamma_{jk} \alpha_k = \sum_{k=1}^n \gamma_{jk} \xi_k, \quad j = 1, 2, 3, \dots, m+1$$

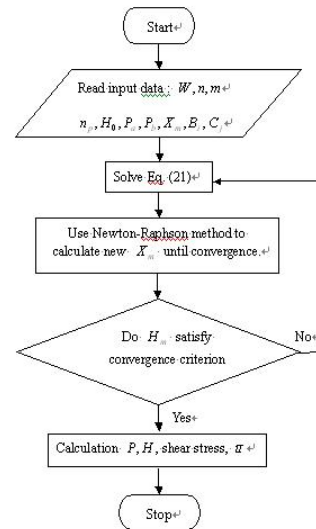
where

$$\beta_{ik} = [X_k^{(i-1)}(2X_k - 1) + (i-1)X_k^{(i-2)}(X_k^2 - X_k)] H_{kb}^3$$

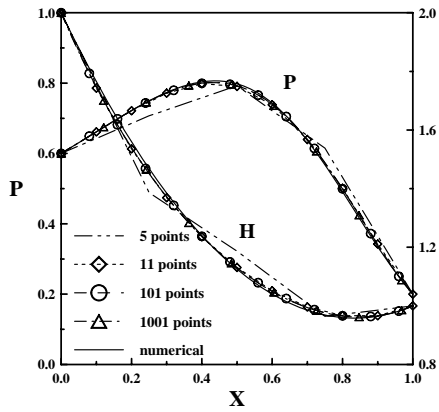
$$\gamma_{jk} = -6X_k^j (X_k - 1)$$

$$\xi_k = 6[(H_0 + 1) - X_k - H_m] + P_a H_{kb}^3$$

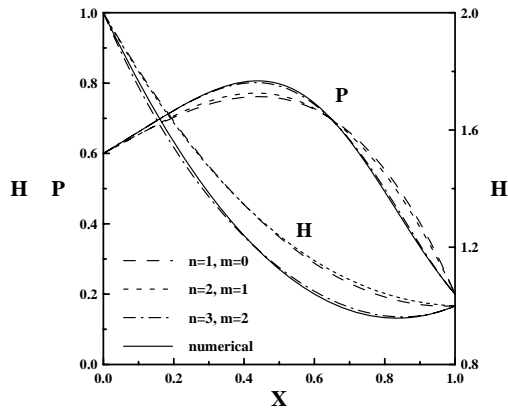
$$\alpha_k = \sum_{i=1}^{n+1} [X_k^{(i-1)}(2X_k - 1) + (i-1)X_k^{(i-2)}(X_k^2 - X_k)] H_{kb}^3 - \sum_{j=1}^{m+1} 6X_k^j (X_k - 1) \quad (20)$$



Results and Discussion (1)

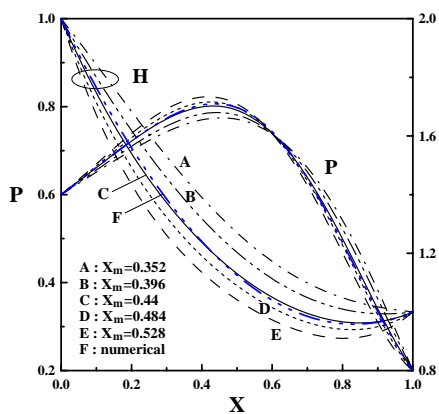


Pressure distributions and film shapes estimated by the present algorithm with different number of points in film thickness

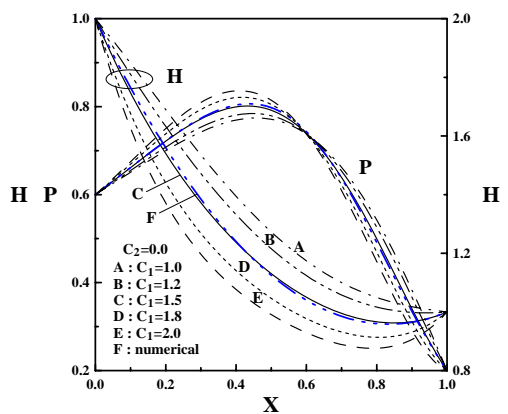


Pressure distributions and film shapes estimated by the present algorithm with different degrees of the polynomial function

Results and Discussion (2)

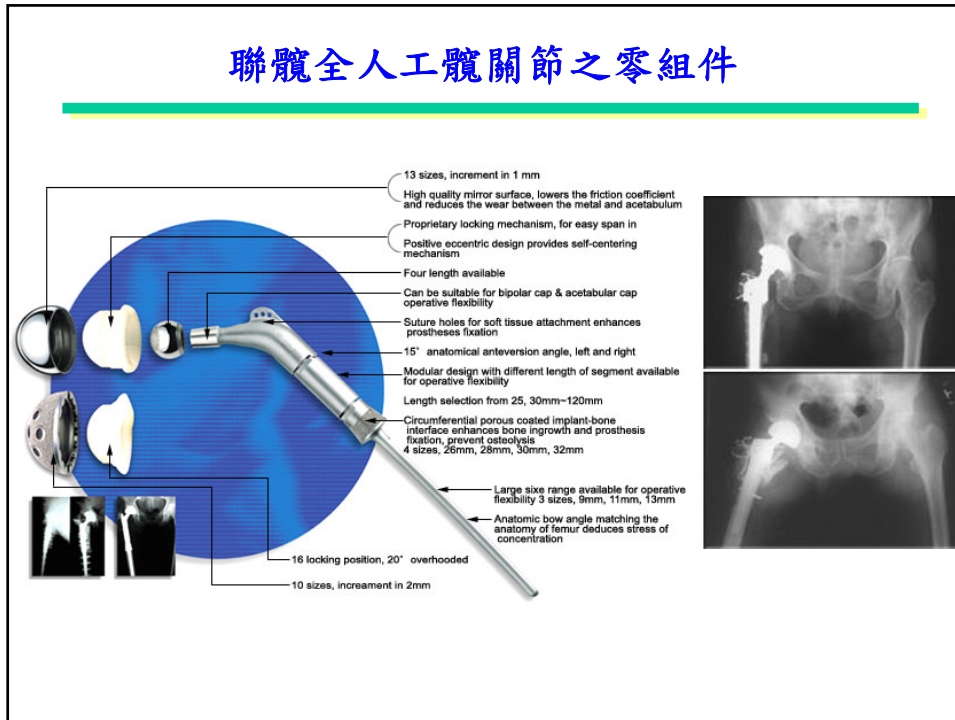


Effect of error in X_m on pressure distributions and film shapes

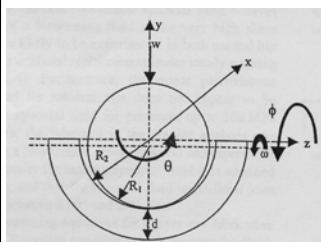


Effect of error in C_j on pressure distributions and film shapes

聯體全人工髖關節之零組件



在球窩關節模型中，以代表人類天然和人工髖關節的軟襯墊預測潤滑膜的厚度



Reynolds equation :

$$\sin \theta \frac{\partial}{\partial \theta} (h^3 \sin \theta \frac{\partial p}{\partial \theta}) + \frac{\partial p}{\partial \phi} (h^3 \frac{\partial p}{\partial \phi}) = 6\eta R_2^2 \omega \sin^2 \theta \frac{\partial h}{\partial \phi}$$

Elasticity equation:

$$h = h_g + \delta$$

$$h_g = c(1 - \epsilon_x \sin \theta \cos \phi - \epsilon_y \sin \theta \sin \phi)$$

$$\delta = \frac{d}{E} (1 - \frac{2\nu^2}{1-\nu}) p$$

Force balance equations:

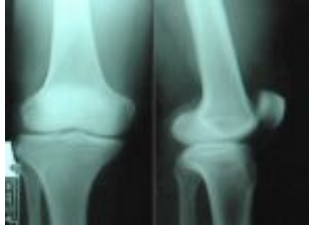
$$F_x = R_2^2 \int_{\phi_1}^{\phi_2} \int_{\theta_1}^{\theta_2} p \sin \theta \cos \phi \sin \theta d\theta d\phi = 0$$

$$F_y = R_2^2 \int_{\phi_1}^{\phi_2} \int_{\theta_1}^{\theta_2} p \sin \theta \sin \phi \sin \theta d\theta d\phi = w$$

$$F_z = R_2^2 \int_{\phi_1}^{\phi_2} \int_{\theta_1}^{\theta_2} p \cos \theta \sin \theta d\theta d\phi = 0$$



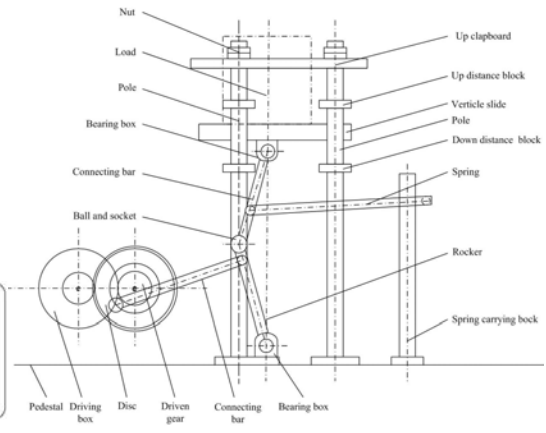
人工關節磨耗試驗機



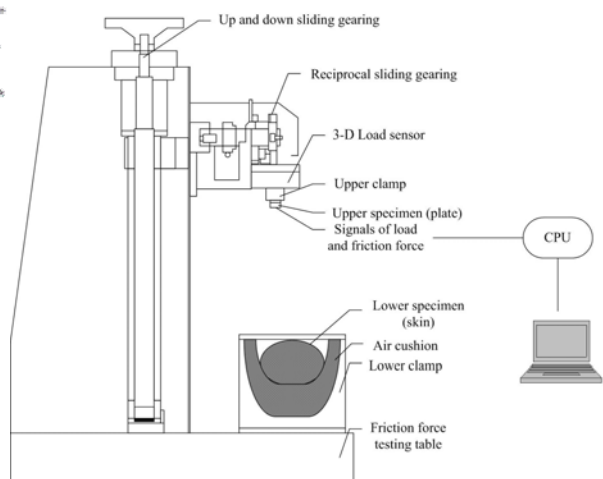
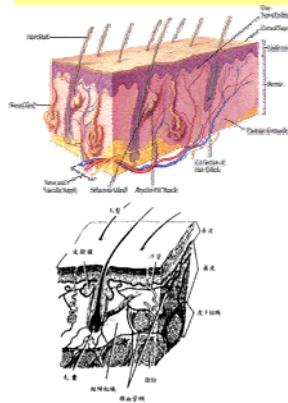
正常的膝關節



人工關節



皮膚摩擦特性量測試驗機



***Thank you for your
attention!***

