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Flow factor approach to molecularly thin hydrodynamic film lubrication

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SUMMARY

Molecularly thin hydrodynamic film lubrication is the mode of lubrication where the lubricating film is molecularly thin and the lubricating media across the film thickness is a molecule instead of the conventional continuum lubricant material. In this lubrication, across the film thickness, the film is a non-continuum due to its molecular thickness while the lubricating molecule is discretely distributed and its behavior is thermohydrodynamic random. The lubricating effect of these molecules is the ensemble average of the behavior of these molecules subjected to shear motion and is determined by the ensemble averaged total flow rate of these molecules through the contact. In this lubrication, the molecular dynamics effect and the non-continuum effect across the film thickness predominantly occur. The molecular dynamics effect includes three components, i.e. viscous, elastic and plastic effects of shear among neighbouring molecules, and the non-continuum effect across the film thickness includes two components, i.e. the fluid discontinuity and inhomogeneity effects across the film thickness. In this lubrication, the molecular dynamics effect and the non-continuum effect across the film thickness can be separated from each other and they can be respectively taken into account in the analysis of this lubrication. It is proposed that in this lubrication the molecular dynamics effect can be described by the dynamic effect of the equivalent continuum lubricant across the film thickness, and the non-continuum effect across the film thickness can be described by the flow factor due to the combined effects of the fluid discontinuity and inhomogeneity across the film thickness for this lubrication as introduced by Zhang [1], by the equivalent transform method. This gives a practical approach to molecularly thin hydrodynamic film lubrication for the theoretical analysis of this lubrication.

Key words: *Molecularly thin hydrodynamic film lubrication, flow factor, molecular dynamics, non continuum, fluid discontinuity, fluid inhomogeneity.*

1. INTRODUCTION

Molecularly thin hydrodynamic film lubrication is now becoming more and more important mode of lubrication. It is the mode of lubrication depending on the physical adsorbed film layer and its ordering to the contact surfaces. This lubrication is now more often seen and becoming one of the most important lubrications in practice. One of the reasons for this is that the operating condition in hydrodynamic lubrication tends to be increasingly severe with the development of modern industry and the lubricating film thickness is consequently increasingly lower with proceeding time and frequently occurs on the nanometer scale in today's industry especially in some advanced mechanical devices. The second reason for this is that the nano-technology makes the mechanical part micro and the lubricating film thickness on this micro mechanical element is usually on the nanometer scale. This mode of lubrication is not new and is actually a mode of boundary lubrication. However, the knowledge of this mode of lubrication is now still relatively small and the theoretical and experimental investigations on this mode of lubrication are now required.

Molecularly thin hydrodynamic film lubrication is a mode of boundary lubrication realized by the physical adsorbed layer film to the contact surfaces. In this lubrication, the lubricating film is molecularly thin and the lubricating film layer is ordered to the contact surfaces. As a result, the lubricating media in this lubrication is a molecule instead of the conventional continuum lubricant. The fluid discontinuity and inhomogeneity effects across the film thickness respectively due to the molecule discrete distribution and ordering across the film thickness thus need to be incorporated in this lubrication. On the other hand, molecular dynamics effect due to molecule shear motion needs to be incorporated in this lubrication. These are two generally important kinds of effects in a real molecularly thin hydrodynamic film lubrication.

The molecular dynamics effect in molecularly thin hydrodynamic film lubrication includes three components, i.e. viscous, elastic and plastic effects of shear among neighbouring molecules in the lubricated contact. It was easily inclined previously to study this effect by molecular dynamics simulation. However, molecular dynamics simulation is not a capable tool for studying the lubricating film rheological behavior showing the molecular dynamics effect in molecularly thin hydrodynamic film lubrication. It can only give some insights into some of the lubricating film physical properties in shear relevant to this lubrication, but it is far away from giving a practical lubricating film rheological model for this lubrication which shows the molecular dynamics effect.

2. PROBLEM DESCRIPTION

Zhang [2], [3], [4] proposed that in molecularly thin hydrodynamic film lubrication the molecular dynamics effect can be described by the dynamic effect of the equivalent continuum lubricant across the film thickness, which also shows the viscous, elastic and plastic effects of shear within the lubricating film. He proposed that in molecularly thin hydrodynamic film lubrication this equivalent continuum lubricant be modelled by the following continuum lubricant viscoelastic and plastic rheological model, to incorporate the molecular dynamics effect:

$$\begin{cases} \dot{\gamma} = \dfrac{1}{G^{eff}_{ncf}(p,h)}\dfrac{d\tau}{dt} + \dfrac{1}{\eta^{eff}_{ncf}(p,h)}\tau_0(p,h)\sinh\left[\dfrac{\tau}{\tau_0(p,h)}\right], & for\ |\tau| < \tau_l(p,h) \\ \tau = sign(\dot{\gamma})\tau_l(p,h), & for\ |\tau| \geq \tau_l(p,h) \end{cases} \tag{1}$$

Here, $\tau_0(p,h)=\tau_{l,ncf}(p,h)/2.8$; $\tau_{l,ncf}$ is the shear strength of this equivalent lubricant. Within the lubricating film $\tau_l(p,h)=\tau_{l,ncf}(p,h)$, while at the lubricating film-contact interface $\tau_l(p,h)=\tau^i_{l,ncf}(p,h)$ ($\tau^i_{l,ncf}$ is the shear strength of this interface). Equation (1) describes the dynamic behavior of this equivalent continuum lubricant in shear and then the molecular dynamics effect in molecularly thin hydrodynamic film lubrication if the lubricant property parameters in this equation are properly expressed.

The rheological properties of this equivalent lubricant in Eq. (1) and the parameter $\tau^i_{l,ncf}$ are respectively expressed in the following, according to Zhang [2, 3]:

$$\begin{aligned} \eta^{eff}_{ncf}(p,h) &= Cy(h)\eta_{cf}(p) \\ G^{eff}_{ncf}(p,h) &= Cg(h)G_{cf}(p) \\ \tau_{l,ncf}(p,h) &= Ctaol(h)\tau_{l,cf}(p) \\ \tau^i_{l,ncf}(p,h) &= Ctaol^i(h)\tau^i_{l,cf}(p) \end{aligned} \tag{2}$$

Here, η_{cf}, G_{cf}, $\tau_{l,cf}$ and $\tau^i_{l,cf}$ are corresponding parameters for the same p value when this lubricant is a continuum; Cy, Cg, $Ctaol$ and $Ctaol^i$ are respectively dimensionless ratios. The dependences of $Cy(h)$, $Cg(h)$, $Ctaol(h)$ and $Ctaol^i(h)$ are expressed by the following general equation, according to Zhang [2]:

$$C(h) = \begin{cases} 1, & for\ \dfrac{h}{h_{cr,ncf}} \geq 1 \\ \displaystyle\sum_{j=0}^{N} \alpha_j \left(\frac{h}{h_{cr,ncf}}\right)^{-j}, & for\ r \leq \dfrac{h}{h_{cr,ncf}} < 1 \end{cases} \tag{3}$$

where N is a positive integral; α_j (for $j=0, 1, \ldots, N$) is a constant; $h_{cr,ncf}$ is a critical thickness of the non-continuum lubricant film, above which the lubricant may be considered to be continuous across the film thickness. According to Zhang [2], the dimensionless parameters in Eq. (3) are shown in Table 1.

Table 1 The dimensionless parameters in Eq. (3) for ratios Cy, Cg, Ctaol and Ctaol^i

	N	α_j	r
Cy	Ny	a_j	$\to 0$
Cg	Ng	b_j	β_0
$Ctaol$	$Ntaol$	d_j	β_0
$Ctaol^i$	$Ntaol^i$	d^i_j	β_0

β_0 is a contact adhering layer constant.

The density (ρ_{ncf}^{eff}) and solidification pressure ($p_{s,ncf}^{eff}$) of this equivalent continuum lubricant are expressed as follows, according to Zhang [2]:

$$\rho_{ncf}^{eff}(p,h) = Cq(h)\rho_{cf}(p) \quad \text{and} \quad p_{s,ncf}^{eff}(h) = Cps(h)p_{s,cf}^{0} \tag{4}$$

where ρ_{cf} is the density of the continuum lubricant given for the same value of p; $p_{s,cf}^{0}$ is the solidification pressure of the continuum lubricant (and constant for isothermal lubrication). Values *Cq* and *Cps* are dimensionless ratios, respectively, expressed as the following:

$$Cq(h) = \begin{cases} 1 & , for \ \dfrac{h}{h_{cr,ncf}} \geq 1 \\ \displaystyle\sum_{j=0}^{Nq} q_j \left(\frac{h}{h_{cr,ncf}} \right)^j & , for \ 0 < \dfrac{h}{h_{cr,ncf}} < 1 \end{cases} \tag{5}$$

$$Cps(h) = \begin{cases} 1 & , for \ \dfrac{h}{h_{cr,ncf}} \geq 1 \\ -\left(\dfrac{1 - h/h_{cr,ncf}}{1 - \beta_0} \right)^n + 1 & , for \ \beta_0 \leq \dfrac{h}{h_{cr,ncf}} < 1 \end{cases}$$

Here, *Nq* is a positive integral; q_j (*for j=0,1, …, Nq*) is *a* constant; *n* is a constant.

In a hydrodynamic lubrication, when the lubricating film thickness is over the critical thickness of the non-continuum lubricating film, the molecular dynamics effect becomes the dynamic effect of the continuum lubricating film, which is described by Eq. (1). In this case, the rheological properties of the equivalent continuum lubricant given above becomes the rheological properties of the actual (continuum) lubricant. It is a limiting case of the definition of the equivalent continuum lubricant for molecularly thin hydrodynamic film lubrication.

Molecular dynamics simulation can play a role in evaluating the rheological properties of the equivalent continuum lubricant given above for a molecularly thin hydrodynamic film lubrication and judging appropriate values of the parameters tabulated in Table 1 respectively for *Cy*, *Cg*, *Ctaol* and $Ctaol^i$ and appropriate values of the parameters respectively for *Cq* and *Cps* shown in Eq. (5) in this lubrication. An example of the values of these parameters for the equivalent continuum lubricant for a molecularly thin hydrodynamic film lubrication is shown in Tables 2 and 3, according to Zhang and Lu [4].

Zhang [1, 2, 3, 5] showed that in a molecularly thin hydrodynamic film lubrication the non-continuum effect across the film thickness i.e. the fluid discontinuity and inhomogeneity effects across the film thickness can be separated from the molecular dynamics effect. Considering the viscous effect of shear among neighbouring molecules in the lubricated contact and the contact-adhering layer interfacial slip, Zhang [1] derived an exemplary expression for the flow factor (θ_v) which is used to correct the total flow rate of the equivalent continuum lubricant described above through the contact to calculate the real total flow rate of the (non-continuum) lubricant through the contact in one-dimensional molecularly thin hydrodynamic film lubrication, due to the combined effects of the fluid discontinuity and inhomogeneity across the film thickness in this lubrication. His defined flow factor reflects the fluid discontinuity and inhomogeneity effects across the film thickness on the total flow rate of the lubricant through the contact in one-dimensional molecularly thin hydrodynamic film lubrication. This flow factor is very important for obtaining the governing flow equation i.e. Reynolds equation for one-dimensional molecularly thin hydrodynamic film lubrication considering the combined effects of the fluid discontinuity and inhomogeneity across the film thickness in this lubrication. It is generally used in the realistic theoretical analysis of this lubrication.

An exemplary expression of this flow factor (θ_v) was given by Zhang [1] for one-dimensional molecularly thin hydrodynamic film lubrication to be:

$$\theta_v = \frac{1 + K(F_1 - F_2)}{1 - K} \tag{6}$$

where the ensemble characteristic parameters F_1 and F_2 of the non-continuum film across the film thickness and the operational parameter *K* are respectively expressed by the equations in Zhang's paper [1]. The values of the ensemble characteristic parameters F_1 and F_2 of the non-continuum film across the film

Table 2 Values of the dimensionless parameters in the equivalent continuum lubricant property parameter expressions for a molecularly thin hydrodynamic film lubrication (a) [4]

Parameter	*Ny*	a_0	a_1	a_2	*Ng*	b_0	b_1	b_2	*Ntaol*	d_0	d_1	d_2
Value	*2*	*1.0822*	*-0.1758*	*0.0936*	*2*	*0.9725*	*0.0262*	*1.2573E-3*	*2*	*0.9726*	*0.0261*	*1.3158E-3*

Table 3 Values of the dimensionless parameters in the equivalent continuum lubricant property parameter expressions for a molecularly thin hydrodynamic film lubrication (b) [4]

Parameter	$Ntaol^i$	d_0^i	D_1^i	d_2^i	*Nq*	q_0	q_1	q_2	q_3	*n*	b_0
Value	*2*	*0.9726*	*0.0261*	*1.3158E-3*	*3*	*1.30*	*-1.0654*	*1.3361*	*-0.571*	*5.4623*	*0.05*

thickness in Eq. (6) respectively depend on the fluid molecule diameter, the number of the fluid molecules across the film thickness, and the separation and the line viscosity between the neighbouring fluid molecules across the film thickness as shown in Zhang's paper [1]. The value of the operational parameter K in Eq. (6) depends on the film pressure gradient, the film thickness, the bulk viscosity of the fluid, the contact-adhering layer interfacial slip rate, and the speeds of the upper and lower contact surfaces at the location where this K value is calculated, as shown in Zhang's paper [1].

The above flow factor is based on the model of the molecularly thin lubricating film in one-dimensional contact shown in Figure 1(b). In this model, the fluid molecule is assumed to be rigid balls. The fluid molecules are assumed to be ordered in the direction normal to the contact surfaces. The fluid discontinuity across the film thickness is expressed by $\Delta_{i+1}/\Delta_i=q_0>1$ (for $i=0, 1, \ldots, (n-1)/2-2$), where n is the number of the fluid molecules across the film thickness and assumed to be an odd number, i is the order number of the fluid molecule across the film thickness, ($(n-1)/2$ is the order number of the fluid molecule at the median plane of the fluid film across the film thickness), Δ_i is the separation between the i-th and $(i+1)$-th fluid molecules across the film thickness, and the ratio q_0 is the equivalent constant ratio between the neighbouring fluid-molecule separations across the film thickness. The line viscosity $\eta_{line,i}$ between the neighbouring fluid molecules across the film thickness satisfies $\eta_{line,i}/\eta_{line,i+1}=q_0^m$ (for $i=0, 1, \ldots, (n-1)/2-2$), where m is the equivalent constant exponent. In this model, the fluid inhomogeneity across the film thickness is expressed by the variations of the separation Δ_i and the line viscosity η_{line} between the neighbouring fluid molecules across the film thickness. This fluid inhomogeneity is determined by both the value of the exponent m and the average value q_0 of the ratio between the neighbouring fluid-molecule separations across the film thickness. In this model, the separation between the neighbouring fluid molecules across the film thickness is determined by the two parameters Δ_{im} and q_0, where $im=(n-1)/2$ and im is the order number of the fluid molecule at the median plane of the fluid film across the film thickness, and Δ_{im} is the separation between the imth and $(im+1)$-th fluid molecules across the film thickness (at the median plane of the fluid film). The ratio Δ_{im}/D is the main parameter to characterize the fluid discontinuity across the film thickness and its value measures the degree of this fluid discontinuity while D is the fluid molecule diameter. In this model, if $m=1$, only the two parameters q_0 and Δ_{im}/D are needed to describe both the fluid inhomogeneity and discontinuity across the film thickness. Equation (6) is based on the condition $m=1$.

The actual case of a one-dimensional molecularly thin hydrodynamic film lubrication may deviate from the model shown in Figure 1(b). In an actual case of this lubrication, the fluid molecule may be not rigid balls, the fluid molecules may be not ordered in the direction normal to the contact surfaces but ordered along a nonlinear curve with their orientation angles (θ) to the contact surfaces, which are not equal to $90°$. An actual one-dimensional molecularly thin hydrodynamic film lubrication may be like as Figure 1(a) shows. In spite of these deviations, for steady-state condition, an actual one-dimensional molecularly thin hydrodynamic film lubrication can usually be equivalently transformed into the model shown in Figure 1(b) by equivalent transformation method. For an actual one-dimensional molecularly thin hydrodynamic film lubrication, the values of n, m, Δ_{im}/D and q_0 of its equivalent model shown in Figure 1(b) depend on the operating condition. How to accurately determine these values according to the operating condition can be found by molecular dynamics simulation.

When the equivalent model shown in Figure 1(b) for an actual one-dimensional molecularly thin hydrodynamic film lubrication is obtained by transformation and the values of the parameters n, m, Δ_{im}/D and q_0 in this model are calculated, the flow factor θ_v can be calculated according to the approach shown in Zhang's paper [1]. This flow factor is then used for calculating the real total flow rate (q) of the layer film through the contact in a one-dimensional molecularly thin hydrodynamic film lubrication according to the following equation:

$$q=\theta_v \cdot q_{con} \tag{7}$$

where q_{con} is the total flow rate of the equivalent continuum lubricant through the contact in this lubrication for this non-continuum layer film described in the former texts. One of the examples of the application of Eq. (7) is shown in Zhang's paper [3].

Zhang calculated the flow factor θ_v for one-dimensional molecularly thin hydrodynamic film lubrication only by considering the viscous dynamic effect of shear between neighbouring fluid molecules. However, the elastic dynamic effect of shear among neighbouring fluid molecules on the flow factor θ_v may be small, since this effect has a small influence on the total fluid flow through the contact in a hydrodynamic lubrication as conventionally known. Also, the plastic dynamic effect of shear between neighbouring fluid molecules is not considered by him. This effect may occur when the shear stress within the layer film exceeds the limiting shear strength of the layer film in this lubrication. In a one-dimensional molecularly thin hydrodynamic film lubrication, if the plastic dynamic effect of shear within the layer film is ignored, the flow factor θ_v derived by Zhang [1] for this lubrication may be widely applicable in the theoretical analysis of this lubrication. One of the examples of this application is shown in Zhang's papers [3, 4].

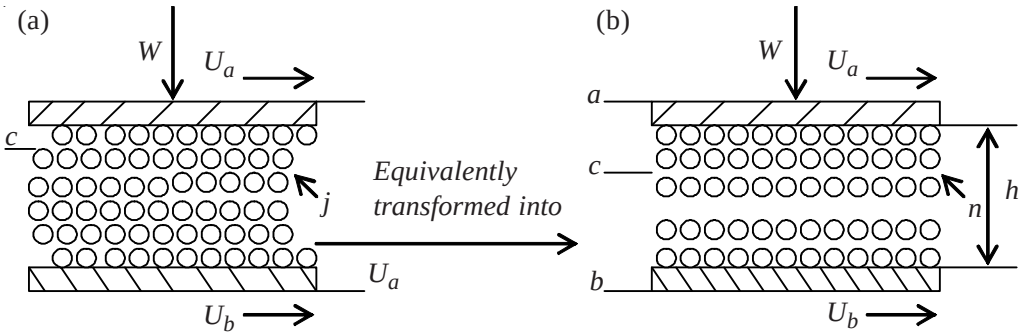

Fig. 1 Molecularly thin adhering layer film in one-dimensional contact: (a) Physical adsorbed boundary film layer ordering to the contact surfaces in a practical contact; (b) Equivalent boundary film layer in the contact of Zhang's model [1]. Explanation of symbols: a - upper contact surface, b - lower contact surface, c - fluid molecule, U_a - speed of the upper contact surface, U_b - speed of the lower contact surface, W - external applied load on the contact, j - number of fluid molecules across the film thickness in a real contact, n - equivalent number of fluid molecules across the film thickness in the contact according to the equivalent transformation method, h - film thickness

3. CONCLUSION

The conclusion is that two types of important effects need to be considered in the analysis of molecularly thin hydrodynamic film lubrication. They are the molecular dynamics effect and the non-continuum effect across the film thickness. They can be separated from each other in a theoretical analysis of this lubrication. The molecular dynamics effect can be described by the dynamic effect of the equivalent continuum lubricant across the film thickness, and the non-continuum effect across the film thickness can be described by the flow factor θ_v due to the combined effects of the fluid discontinuity and inhomogeneity across the film thickness for this lubrication as introduced by Zhang [1], by the equivalent transformation method. These form an applicable approach to molecularly thin hydrodynamic film lubrication. In the further derivation for the flow factor θ_v, the elastic dynamic effect of shear among neighbouring molecules in this lubrication needs to be considered. Molecular dynamics simulation can play a role in evaluating the rheological properties η_{ncf}^{eff}, G_{ncf}^{eff}, ρ_{ncf}^{eff}, $\tau_{l,ncf}^{eff}$, $p_{s,ncf}^{eff}$ of the equivalent continuum lubricant in this lubrication and in accurately determining the values of n, m, Δ_{im}/D and q_0 of the equivalent model shown in Figure 1(b) of a molecularly thin hydrodynamic film lubrication.

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PRISTUP MOLEKULARNO TANKOM HIDRODINAMIČKOM SLOJU PODMAZIVANJA POMOĆU FAKTORA TOKA

SAŽETAK

Molekularno tanki hidrodinamički sloj podmazivanja je način podmazivanja u kojemu je sloj podmazivanja molekularno tanak, a medij podmazivanja kroz debljinu sloja je molekula umjesto uobičajenog neprekidnog materijala za podmazivanje. U ovakvom podmazivanju, kroz debljinu sloja, sloj nije neprekinut zbog svoje molekularne debljine dok je podmazujuća molekula diskretno raspoređena, a njeno ponašanje je termodinamički nepravilno. Efekt podmazivanja ovih molekula dan je općim prosječnim ponašanjem molekula izloženih tangencijalnom gibanju, a određuje se pomoću sveukupne prosječne brzine toka ovih molekula kroz dodir. U ovakvom podmazivanju uglavnom se pojavljuju efekti molekularne dinamike i prekinutosti kroz sloj debljine. Efekt molekularne dinamike sadrži tri komponente, tj. viskozna, elastična i plastična djelovanja posmika između susjednih molekula, a efekt prekinutosti kroz debljinu sloja uključuje dvije komponente: fluidni diskontinuitet i efekte nehomogenosti kroz debljinu sloja. U ovom podmazivanju, djelovanje molekularne dinamike i djelovanje prekinutosti kroz debljinu sloja mogu se odvojiti jedan od drugoga i uzeti u obzir u analizi podmazivanja. Predlaže se da se u ovom podmazivanju molekularno dinamičko djelovanje opiše pomoću dinamičkog djelovanja ekvivalentnog neprekinutog maziva kroz debljinu sloja, a djelovanje prekinutog kroz debljinu sloja može se opisati faktorom toka zbog kontinuiranih djelovanja fluidnog diskontinuiteta i nehomogenosti kroz debljinu sloja za ovo podmazivanje, kao što je naveo Zhang [1], pomoću ekvivalentne metode transformacije. Ovim je dan jedan praktičnan pristup molekularno tankom hidrodinamičkom sloju podmazivanja u teorijskoj analizi podmazivanja.

***Ključne riječi**: molekularno tanki hidrodinamički sloj podmazivanja, faktor toka, molekularna dinamika, prekinutost, diskontinuitet fluida, nehomogenost fluida.*