Applied Mathematical Modelling 37 (2013) 406–419

Contents lists available at SciVerse ScienceDirect

Applied Mathematical Modelling

journal homepage: www.elsevier.com/locate/apm

Thin film tribology of pharmaceutical elastomeric seals

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ARTICLE INFO

Article history:
Received 22 April 2011
Received in revised form 6 February 2012
Accepted 29 February 2012
Available online 8 March 2012

Keywords:
Pressurised metered dose inhaler
Elastomeric pharmaceutical seals
soft Ehl
Siliconisation

ABSTRACT

The primary purpose of valve seals in inhalation and other drug dispensing devices is to inhibit leakage of highly volatile formulation from pressurised canisters. This requirement often conflicts with smooth operation of valves because of poor lubrication of seals. The repercussions of this can be variability in dispensed dose as well as loss of prime and gradual wear of seals. Although a good volume of literature is available for general purpose o-ring seals, the characteristic behaviour of those used in pharmaceutical devices deviate from this significantly. The paper studies tribology of such seals, subjected to global fitment and canister pressure deformation and localised conjunctional elastohydrodynamic pressures. It is shown that ideally smooth seals would operate under iso-viscous elastic (*soft EHL*) regime of lubrication. However, the predicted ultra-thin films are insufficient to ensure fluid film lubrication because of rough micro-scale nature of elastomeric seal surface and poor lubricity of the usual bio-compatible formulations. The paper also shows that siliconisation of elastomeric contacting surface only marginally improves its tribological performance.

1. Introduction

Many inhalation devices contain drug formulations (mixtures) which are volatile and kept in metering chambers under pressure. Sealing of the chamber is a primary design requirement. Smooth actuation of the device is also an important design attribute, which can often conflict with its primary sealing requirement. This calls for the use of a bio-compatible lubricant, a desired property of the propellant which accounts for the main constituent of the mixture. This is the characteristic of chlorofluorocarbon (CFC), which was abandoned after its undesired effect upon the ozone layer was recognised. Instead many inhalation devices now use hydrofluoroalkane (HFA)-based propellants which interact minimally with the surfaces of the chamber and the seals because of its inert nature [1]. HFA, however, suffers from very poor lubricity. As the result, the elastomeric seals for pharmaceutical device applications are often furnished with a film of silicone oil (a process referred to as siliconisation). With HFA being the propellant of choice, only certain types of elastomeric seals may be used. Thus, in a variety of applications where elastomers are the main sealing elements, such as pressurised metered dose inhalers (pMDIs) and syringes, the seal performance represents the main contributory factor to the overall system friction. Whilst reducing friction is a desired outcome, it should not compromise the primary sealing function.

It is only recently that some research effort has been directed towards tribology of elastomeric seals in pharmaceutical devices [2,3]. However, research into pharmaceutical seals inherits a larger volume of general research on seal tribology. One key issue has been the prediction of contact pressure distribution and thus the conjunctional load in order to assess

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http://dx.doi.org/10.1016/j.apm.2012.02.035

Nomenclature

b	width of effective seal contact
c	seal undeformed half face-width
D	seal cross-sectional diameter (undeformed)
E	elastic modulus of EPDM rubber
E_p	elastic modulus of Polybutylene Terethalate
E'	equivalent elastic modulus of the contact
h	film thickness
h_0	minimum film thickness (rigid gap)
H	dimensionless film thickness
H_0	dimensionless minimum film (gap)
i	position along the face-width where deflection is calculated
j	an iteration counter
k	position of a pressure element
l	perimeter of the seal
n	number of discrete computational elements
p	elastohydrodynamic contact pressure
P	load per unit computational element width
P_H	equivalent Hertzian pressure
p^*	dimensionless contact pressure
R	cross-sectional seal radius
R_1	radius of the undeformed seal before fitment
R_2	radius of the rectangular groove
R_{zy}	equivalent radius of contact
S	face-width profile of the seal
u	speed of lubricant entraining motion
w	contact load
U^*	dimensionless speed parameter (rolling viscosity parameter)
W^*	dimensionless load parameter
x	normal to the seal cross-section
y	along the seal face-width
Y_e	exit boundary (Film rupture point)
Y_i	inlet meniscus
z	along the cross-section of the seal
α	pressure viscosity coefficient of lubricant
β	relaxation constant for fitment load per unit length
χ	under relaxation factor for elasto-hydrodynamic pressures
δ	localised deflection of the seal
Δ	global seal deflection due to fitment and canister pressure
$\bar{V}$	dilatation
ε_f	error in fitment extension
ε_{p^*}	error in elastohydrodynamic pressure convergence
ε_y, ε_z	cross-sectional strains
γ	shear strain
η	dynamic viscosity at contact pressure
η_0	dynamic viscosity at atmospheric pressure
ρ	density at contact pressure
ρ_0	density at ambient pressure
σ_y, σ_z	principal stresses
τ_{zy}	shear stress
υ	Poisson's ratio for EPDM rubber
υ_p	Poisson's ratio for Polybutylene Terethalate
ζ	damping factor for convergence of lubricant reaction

sealing effectiveness. The first step in this process is the accurate prediction of contact geometry when a seal is fitted *in situ* and is subjected to a differential pressure.

The initial approaches involved use of Hertzian theory for o-ring seals to represent their localised deformation in one dimensional analysis, when they are loaded against their retaining grooves. However, Hertzian theory does not take into