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A weak-inertia mathematical model of bubble growth in a polymer foam

Euan Barlow[a,b,*], Aoibhinn M. Bradley[a], Anthony J. Mulholland[a], Carmen Torres-Sanchez[c]

[a] Department of Mathematics and Statistics, University of Strathclyde, Glasgow, G1 1XH, UK
[b] Department of Management Science, University of Strathclyde, Glasgow, G4 0GE, UK
[c] Wolfson School of Mechanical, Electrical and Manufacturing Engineering, Loughborough University, Loughborough, LE11 3TU, UK

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ABSTRACT

One possible manufacturing method for bone scaffolds used in regenerative medicine involves the acoustic irradiation of a reacting polymer foam to generate a graded porosity. This paper derives a mathematical model of a non-reacting process in order to develop theoretical confirmation of the influence of the acoustic signal on the polymer foam. The model describes single bubble growth in a free rising, non-reacting polymer foam irradiated by an acoustic standing wave and incorporates the effects of inertia. Leading and first order asymptotic inner solutions in the temporal domain (early growth) are presented for the case of instantaneous diffusion when the fluid volume surrounding the bubble is large compared to the bubble volume. The leading order asymptotic outer solution (late growth), for the case of instantaneous diffusion, is described analytically using the Picard iteration method. Initial conditions for this outer solution are identified through matching with the asymptotic inner solution. A numerical solution for the leading order outer equation is also presented. Investigations are carried out to explore the influence of inertia on the bubble volume, fluid pressure and the stress tensors of the foam, and to explore the effect of fluid viscosity and acoustic pressure amplitude on the final bubble volume, and the curing time. A key result is that increasing the applied acoustic pressure is shown to result in a reduced steady state bubble volume, indicating that ultrasonic irradiation has the potential to produce tailored porosity profiles in bioengineering scaffolds.

1. Introduction

1.1. Motivation

A polymeric foam is a particular example of a viscoelastic, heterogeneous material which is composed of at least two phases (one solid plus voids whose size distribution can be varied [43]). Bone scaffolds [43] are the biocompatible materials which provide the support structure for the growth of tissue engineered bone precursors [8,20]. The physical properties of polymeric foams make these particularly suitable for bone scaffold applications, including their low density, chemical inertness, high wear resistance, biodegradability and thermal and acoustic insulation. One of the factors contributing to the strength and functionality of natural bone is its functionally graded porosity, with higher density on the periphery of the structure and higher porosity at the centre [6]. The best grafts and bone substitutes are considered to be those with biomechanical and biological properties most closely resembling the non-uniform graded porosity distribution observed in natural bone [6], and it is therefore desirable to mimic this property.

A number of different approaches to the tailored design and manufacture of bone scaffolds have been reported, including control of the processing conditions and of the chemical composition of the polymer material [9,40,48]. Ultrasonic irradiation of liquids has been shown experimentally to result in a number of unusual phenomena including rectified diffusion and increased polymerisation reaction rate [19,22,32,42]. Torres-Sanchez and Corney [43] developed an empirical method for designing bone scaffolds, which uses an acoustic standing wave to irradiate a sample of polymerising polyurethane foam to tailor the porosity profile within the final cured sample to a particular porosity specification. A relationship between the pressure amplitude of the irradiating sound wave and the porosity value at a given position in the sam-

* Corresponding author:
E-mail address: euan.barlow@strath.ac.uk (E. Barlow).

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ple was demonstrated experimentally. Ultrasound was observed to have an impact at particular stages during the reaction, and the authors hypothesized that this was due to the fact that diffusion and convection were predominant effects during these stages.

This paper presents the first attempt at mathematically modelling the experiment presented by Torres Sanchez and Corney [43] and the key mechanisms involved in this complex reaction, to develop an understanding of this process and provide the first steps towards supporting the production of strictly defined and controlled porosity profiles. Polymerisation is a complex process involving factors such as bubble dynamics, evolving rheology [16,28], a two-phase fluid, rectified diffusion [10–13,25], Bjerknes forces [3,23] and Ostwald ripening [27,35]. Of additional relevance in this study is the effect of the ultrasonic irradiation. To make headway with modelling this complex process, concentration is focused on the post nucleation evolution of a bubble in a viscoelastic fluid and the effects of rectified diffusion, Bjerknes forces and Ostwald ripening are ignored. The effect of the ultrasound pressure amplitude on the long term growth of the bubble is, however, considered. The effects of inertia are incorporated into the model as it plays a significant role in the early stages of the bubble's evolution.

1.2. Bubble dynamics

Much work has been done to study and model the nucleation [18,36,38] and subsequent single bubble growth [5,14–18,30,37–39,41,45] in viscoelastic materials including polymer foams, both reacting [16] and non-reacting [14–17,49]. The effects of ultrasound on nucleation [50] and subsequent growth of a single bubble via rectified diffusion in an aqueous fluid [24,26,29,33,34] have been studied extensively.

There have been a number of studies of the nucleation and subsequent growth of a single spherical gas bubble in a surrounding fluid due to diffusion of gas through the fluid and into the bubble. Amon and Denson [4] proposed a cell model for the analysis of bubble growth in an expanding polymer foam with each cell containing a spherical gas bubble surrounded by a concentric liquid envelope containing a limited supply of gas. Their model takes account of heat transfer and inertia and couples bubble growth to the changing foam density. Street et al. [39] and Ting [41] both used the Oldroyd B fluid model to describe the viscoelasticity of the surrounding fluid layer which they assumed to be infinite. This resembles the case of early time foaming where bubble size is small and bubbles are spaced at large distances from each other, remaining spherical and not interfering with each other. They demonstrated that the viscoelasticity of the melt as well as the diffusivity of the gas determined the initial growth rate. Arefmanesh and Advani [5] considered the case of a spherical gas bubble surrounded by a finite shell of viscoelastic fluid which they modelled using the upper convected Maxwell model. They introduced a Lagrangian transformation to describe the moving bubble/liquid interface and substituted a concentration potential to aid numerical solution. Their model serves to describe the case where a large number of bubbles exist in close proximity to each other, which can be expected in an expanding polymer foam. Shafi and co-workers [36,37] looked at bubble growth in polymer foams in conjunction with nucleation and concluded that the most sensitive parameters to final bubble size distribution are those associated with nucleation. They found that while growth dynamics can alter the distribution this is only a secondary effect. Feng and Bertelo [18] also looked at the effect of nucleation but proposed a model for heterogeneous nucleation and its effect on the final bubble size distribution. Venerus et al. [45] formulate a model of diffusion induced bubble growth in viscoelastic liquids of infinite extent, demonstrating that under various approximations, several previously published models can be derived from their model, and providing comparison between models. In Venerus [44], transport models of diffusion induced bubble growth in viscous liquids of both finite and infinite extent are developed and evaluated, and results compared with Amon and Denson [4] and Arefmanesh and Advani [5]. Both models agree at early stages of the growth process and differ at later stages when the equilibrium bubble radius is approached for the finite liquid model.

Building on the above work, Everitt et al. [16] proposed two models for individual bubble expansion in curing polymer foams. The first model was for bubble growth in a non-reacting polymer foam; the second models the gas production due to the reaction and the evolving rheology of the viscoelastic material in the reacting polymer foam. In each case the evolving fluid is treated as a multimode Oldroyd B system, and the Lagrangian transformation is used to describe the moving bubble boundary. Everitt et al. [16] neglected the effects of inertia since nondimensionalisation of their system results in a very small Reynolds number, and their model does not include an acoustic forcing term.

1.3. Overview

This paper examines the effect of ultrasonic irradiation on the dynamics of a single bubble in an expanding polymer foam. The non-reacting model proposed by Everitt et al. [16] is extended to include the effects of inertia and the effects of a standing acoustic wave sonicating the polymerising sample. The model equations are derived by consideration of an Oldroyd B polymeric fluid [46]. Once the governing equations, initial and boundary conditions are obtained, an instantaneous diffusion assumption is made in order to partially decouple the system. This is then probed in an effort to derive an approximate analytic solution using asymptotic expansions for the case where the bubble volume is much smaller than the surrounding fluid volume. This regime may describe the situation at early time in the polymerising sample when bubbles have just nucleated and are at large distances from each other so that they are effectively surrounded by an infinite fluid volume. An inner and outer asymptotic solution are proposed; the former to first order and the latter to leading order. The accuracy of the first order asymptotic inner solution is discussed before a leading order analytic solution for the outer temporal variable is derived, where the initial conditions for this outer solution are generated through matching with the asymptotic expansion of the inner solution. A numerical scheme is produced to test the accuracy of the analytic outer solution and the limitations of the analytic solution are discussed before using the numerical scheme to predict the effects of changing viscosity and acoustic pressure amplitude on the outer solution.

Section 2 presents the derivation of the model of bubble growth in a free rising, non-reacting polymer foam irradiated by an acoustic standing wave and incorporating the effects of inertia. The asymptotic derivation of the inner and outer solutions are given in Sections 3 and 4, respectively. Concluding remarks and areas of future work are discussed in Section 5.

2. Mathematical model of a non-reacting foam

In the non-reacting case a polymeric liquid containing a foaming agent is subjected to a sudden reduction in pressure and foaming commences as the foaming agent comes out of solution [16]. This is a two phase system with the foam considered to be a system of identical, spherical bubbles of gas, each surrounded by a layer of viscoelastic fluid containing a quantity of dissolved gas. The model concerns a single bubble with initial volume, $4\pi u(0)/3 = 4\pi R^3/3$, with bubble radius R and initial gas pressure p_{g0}. The fluid surrounding the bubble is assumed to be