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Reply to the comment by Marques et al. on: “Numerical models of flow patterns around a rigid inclusion in a viscous matrix undergoing simple shear: implications of model parameters and boundary conditions” by N. Mandal, S.K. Samanta and C. Chakraborty ☆

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1. Introduction

In structural geology a large number of studies have dealt with flow mechanics of inclusion-matrix systems over the last couple of decades. Among these one set of investigations derive analytical solutions, whereas another approach is to generate numerical solutions by means of the finite element method (FEM). Both lines of study compare the results with that obtained from analogue experiments.

Two types of flow are known to prevail around a circular inclusion embedded in a viscous matrix undergoing simple shear: one with eye-shaped separatrix and the other with bow-tie-shaped separatrix. Flows with both eye- and bow-tie-shaped separatrix may be obtained from analytical solutions by varying the ratio of simple and pure shear in a general type of deformation (Mandal et al., 2001). However, analytical solutions for only simple shear deformation yield flow only with eye-shaped separatrix geometry. Marques et al. (2005) and Mandal et al. (2005) addressed the issue of development of bow-tie-shaped separatrix around a circular inclusion embedded in a viscous matrix undergoing only simple shear. These studies attempted to resolve the issue using FEM considering two parameters: (1) relative dimension of the inclusion with respect to that of the inclusion-matrix system, and (2) model geometry of the inclusion-matrix system. Both the investigations used FEMLAB for the purpose.

Mandal et al. (2005) reviewed all continuum models and showed under which circumstances a bow-tie-shaped separatrix may arise. However, it appears from the feedback of Marques et al. (2006) that there is a necessity for further elaboration of the principles of finite element modelling of an inclusion-matrix system. The results obtained from FEM should ideally converge only when the associated parameters are uniformly constrained. Differences in the assumptions for FEM experiments would yield diverse results, and may lead to misinterpretation (e.g. Marques et al., 2006). Mandal et al. (2005) presented a number of results based on finite element models, to point out how choice of geometrical parameters and boundary conditions can lead to variability in the flow patterns observed in models. It was not the aim of Mandal et al. (2005) to provide a complete model. In the following sections we address more explicitly how different variables should be considered while running FEM experiments.

2. Basic premises of modelling inclusion-matrix systems

Finite element modelling of a deforming system is primarily based on the continuum mechanics of multiply-connected regions, considering boundary conditions imposed at the contours of desired regions, here (1) the inclusion-matrix boundary (R) and (2) the periphery of the model (B), which is considered as a quadrilateral (Fig. 1). In all studies the condition imposed on R is that the inclusion rotates at a rate half the simple shear. Now, as regards to the model boundary the contour B can be split into B1 and B2 parallel and perpendicular to the shear direction, respectively. In the present context we discuss how a choice of the ratios B1/B2 (A_r), B1 or B2/inclusion diameter (D_r) and conditions at B1, B2 may lead to variability in the flow pattern. Marques et al. (2006) claims that the parameter D_r of Mandal et al. (2005) is confused with

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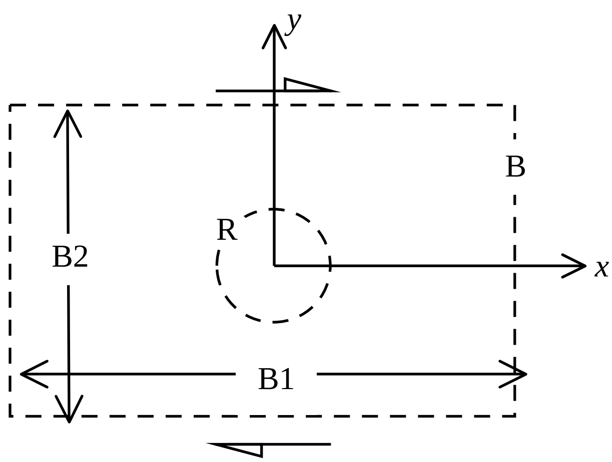

Fig. 1. Consideration of different contours in a multiply connected region. Note that B is the model boundary and R is the inclusion-matrix boundary.

the parameter *S* of Marques et al. (2005), which is a measure of relative model dimension across the shear direction (i.e. B2/inclusion diameter). However, we used D_r with a completely different physical consideration and, therefore, D_r should not be compared with *S* in any way. D_r is a measure of model area (defined by the dimensions both along and across the shear direction) relative to that of the inclusion. This was clearly stated in Mandal et al. (2005).

We reiterate that the model boundaries do not define any physical surface, like the interface between a shear zone and its wall rocks. For example, one may intend to study the structures around a centimetre-scale clast within a shear zone several kilometres wide, where the clast-shear zone thickness ratio would be in the order of 10^6. However, structural geologists usually employ models of smaller dimensions considering the bulk kinematics at the model boundaries, which naturally do not mark any physical boundary, like a shear zone boundary. One aim of Mandal et al. (2005) was to show that model results would depend on the choice of model size relative to that of an inclusion. This is different from the objective of Marques et al. (2005), who intend to show the effect of inclusion dimension relative to shear zone width (with physical boundaries) on the flow pattern around an inclusion, using specific models with length much larger than the width (B1 much greater than B2). On the other hand, Mandal et al. (2005) have chosen model boundaries to show the effect of different model parameters (B1 = B2, B1 > B2, B2 > B1) on the flow pattern obtained in model runs, as commonly done in FEM work.

3. Effects of model parameters

It is understandable that the flow resulting from imposed boundary conditions will depend on the positions of both B1 and B2 with respect to the inclusion. Therefore, the relative distance of B1 (equivalent to the *S* parameter of Marques et al. (2005)) would be necessary, but not sufficient in analyzing the flow in any finite system. We shall show later that the physical feature of flow, e.g. position of stagnation points, for a particular B1 position can vary with changing B2 position (Fig. 1). However, one can keep the position of B2 constant at large distances and show how the flow can change with varying B1 as done by Marques et al. (2005). Mandal et al. (2005) considered models with finite dimensions, as is commonly done (Masuda and Mizuno, 1996; Treagus and Lan, 2003), and has shown the effects of the two geometrical parameters (D_r and A_r) under different dynamic and kinematic conditions imposed at the model boundaries.

Mandal et al. (2005) demonstrated how the streamlines of flow can qualitatively change with increasing lateral dimension of model (B1), while the dimension across the shear direction (B2) remains constant (fig. 7b and c in Mandal et al., 2005). An example is cited here, which shows that the position of stagnation points varies as B1 is changed, while B2 remains unchanged (Fig. 2a). For a given B2, however, the distance of stagnation points does not show any monotonic variation or any particular trend line with increasing lateral dimension of the model. The nature of such variations needs to be further

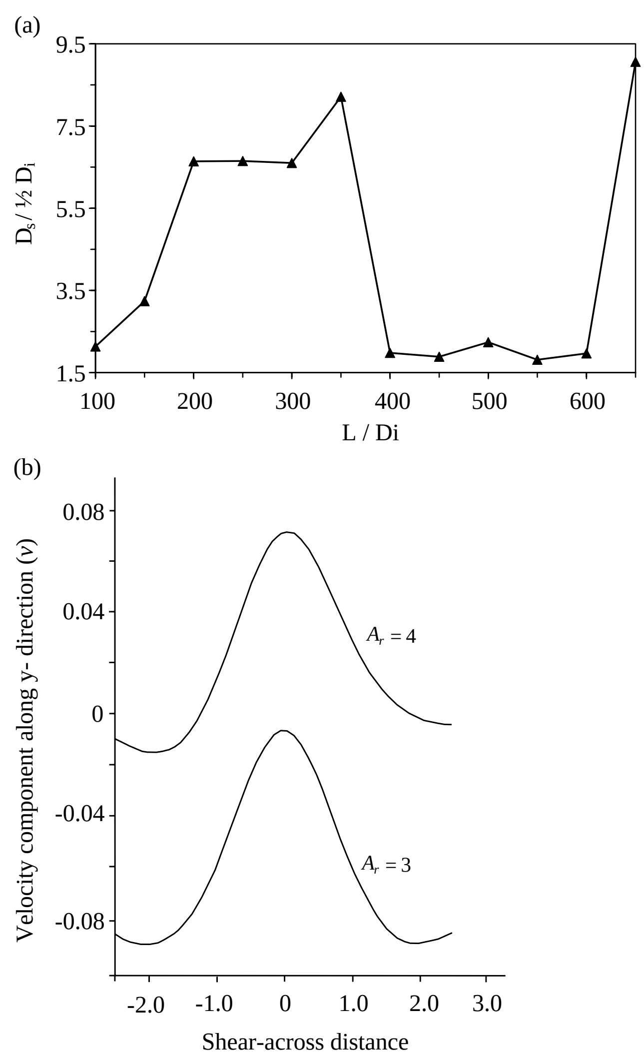

Fig. 2. (a) Plot showing the distance of stagnation points from the centre of inclusion (D_s) with increasing length (*L*) of the model. (b) Profiles of velocity component along the *y*-direction (across shear direction) at $x = -2$ for different aspect ratios (A_r) of model. Inclusion diameter and model width were 1 and 100, respectively. Models were deformed under 'homogeneous simple shear'.

investigated and analyzed from a physical point of view. The ratio B1/B2 will have influence on the flow pattern even when the lateral boundaries are located at a large distance. This is also reflected in the velocity profiles taken at a finite distance from the inclusion (Fig. 2b). For a constant relative model width (i.e. constant *S* of Marques et al., 2005), the profile of *y*-velocity component, for example, significantly varies with increasing model length, i.e. with increasing model aspect ratio. Based on these observations, we concluded that the effect of both the model dimensions in performing numerical experiments should be taken into account. Here we presented results considering a particular type of boundary condition (condition 1: homogeneous shear). Evidently, the effect of shear-along model dimension will be different for different boundary conditions, as shown in Mandal et al. (2005).

4. Concluding remarks

In their comment, Marques et al. (2006) raised some additional points. They claim that fig. 4a of Mandal et al. (2005) is erroneous. However, in this figure the lines with arrows are shown only to represent the direction of particle motion under dextral, homogeneous simple shear without any connotation to the magnitude of velocity vector, as mentioned in the caption. The lines simply show the pattern of streamlines, tangents to which give the instantaneous direction of velocity vectors in space. Marques et al. (2006) misinterpreted the figure, possibly because the arrows are placed at the centre of the streamlines.

We completely disagree with Marques et al. (2006) on the basic principle of shear boxes, which are widely used in soil mechanics and analogue experiments in structural geology. In the conventional set-up of a shear box, model deformation is not imposed by moving only the two plates disposed parallel to the shear direction. In order to attain homogeneous simple shear in the model, all the four sides have to be set in motion (see Ildefonse et al., 1992; Treagus and Sokoutis, 1992). Even in numerical simulations, constant velocity boundary conditions are imposed on all the four boundaries of the model for the shear strain rate to resemble "the situation in a shear-box experiment, where deformation is imposed by movement of rigid boundaries on all sides" (Bons et al., 1997, p. 34; see also Treagus and Lan, 2003). We also disagree with the proposition of Marques et al. (2006) that the lateral walls in a shear box "only serve to avoid collapse of the viscous matrix under its own weight". The purpose of using lateral plates is not only to restrict the lateral flow of the viscous material under gravity, but also to counter-balance the torque of the model developed due to oppositely moving plates. Physical experiments on a viscous block with free lateral faces does not produce homogeneous simple shear strain (Fig. 3), which is also evident from the flow pattern observed in finite element models with the same setup (Dresen, 1991; Mandal et al., 2005).

Marques et al. (2006) is correct in stating that in a ring shear apparatus the shear strain gradient is not homogeneous simple shear as obtained in a square shear box. Generally, in a ring

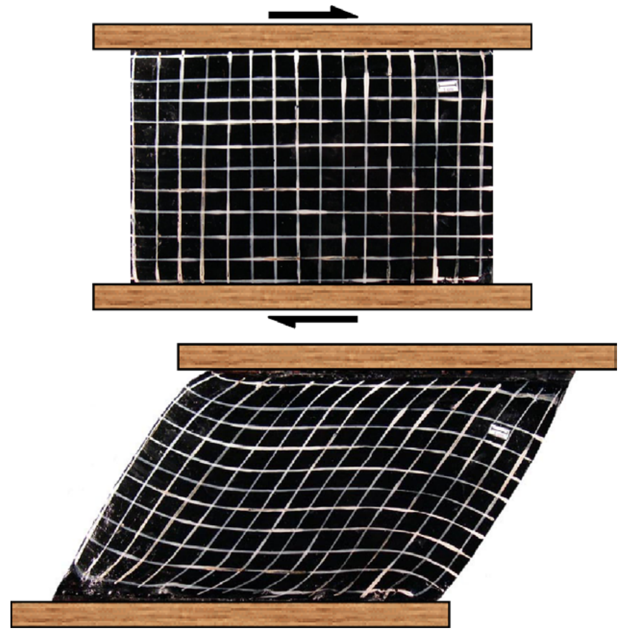

Fig. 3. Physical model experiment with homogeneous rectangular pitch block undergoing dextral shear deformation. The lateral boundaries (left and right) of the model were kept free for simulating unconstrained boundary conditions. Note that the grids are deformed heterogeneously. Scale bar: 1 cm.

shear apparatus only the central part of the model is taken into consideration where the velocity gradient across the shear direction can be assumed to be approximately constant and the straight-out condition prevails as well (Bons et al., 1997).

Marques et al. (2005) state that the length of the model was at least 40 times the diameter of the inclusion. However, they did not provide any information regarding the aspect ratios of individual models in their figs. 7 and 8. Our results indicate that changes in the model shape in Marques et al. (2005) may induce changes in the flow around a rigid inclusion even when the length of the model considerably exceeds the diameter of the inclusion.

Marques et al. (2005) refer to flow in their model as either homogeneous simple shear (section 3.1 and discussion), or as 'straight-out'. However, these two conditions are not identical. The 'straight-out' condition is widely employed for simulating directional fluid flow at the outlet of an open pipe system. This condition does not take into account how the velocity component in the *x*-direction varies in the *y*-direction. The condition only ensures that the fluid does not have a component of motion in the *y*-direction. On the other hand, homogeneous simple shear implies that the velocity in the *x*-direction varies linearly with y, while at the same time there is no velocity component in the *y*-direction. This is the condition that reflects bulk kinematics of large-scale natural shear zones with simple shear and appears to be suitable for simulation of shear zone structures (e.g. Treagus and Lan, 2003). However, the dynamics or kinematic conditions at the lateral boundaries may vary depending on the physical situation and the choice of the modellers (unconstrained—Dresen, 1991; homogeneous shear—Masuda and Mizuno, 1996; Pennacchioni et al., 2000;

Treagus and Lan, 2003; straight-out—Marques et al., 2005). Marques et al. (2006) hinted that the straight-out condition is the most suitable one in models but it is not clear why, either from a modelling or a geological point of view.

In fig. 2a of Marques et al. (2006), they plotted x- and y-velocity components at $x=-1$ keeping the radius of the inclusion as 1. This means that they have chosen a D_R value of 1 instead of 2 and, therefore, their velocity profile lies at the inclusion boundary. However, it is understandable that the velocity profile will depart from linearity, as the deformation at any finite distance from the inclusion is heterogeneous. In this context we must clarify that the boundary condition (homogeneous shear) that we applied at the lateral walls, does not aim to impose the velocity condition produced by the heterogeneous velocity field around the inclusion.

Marques et al. (2006) claim that the flow pattern will always be a bow-tie-shaped separatrix since the “stagnation points must also exist in infinite shear zones, but at an infinite distance to each side of the inclusion”. The assumption that the stagnation points are located at infinity implies that the regime of back flow essentially vanishes and therefore the flow cannot be described ideally as bow-tie shaped.

Finally, the study of Mandal et al. (2005) attempted to show that different model parameters and boundary conditions exert a strong influence and thereby lead to variability in the flow pattern. FEM can therefore only be used taking all these factors in account for analyses with either 2-D or 3-D models.

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