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Comment 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 [Journal of Structural Geology 27 (2005) 1599–1609]

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Flow, rigid inclusion behaviour and associated structures in simple shear have been an important subject of research in structural geology and tectonics in the last two decades for trying to understand kinematics and mechanics of natural ductile shear zones. Previous work by Mandal and co-workers has been of high quality and increased understanding of this issue. However, Mandal et al. (2005) is potentially confusing, because they use boundary conditions that include misconceptions and parameter values that can hardly be found in nature. Our comments on this paper focus on the choice of flow type, boundary conditions and model parameter values, and their implications on the understanding of natural systems.

1. Simple shear flow

Simple shear can be defined as a three-dimensional constant volume flow where dv/dh is constant (v is the velocity along channel length and h is its width) (Fig. 1). A good visualisation of simple shear flow is the sliding of a deck of cards at constant displacement, in which each unstrained card represents particle paths (or stream lines in this case) and the end edges represent the velocity profile. If we agree to this definition, then some of the models in Mandal et al. (2005) are not simple shear flow, and their fig. 4a is misleading because particles do not move at identical velocities in adjacent streamlines as shown in the figure. However, the title of the paper in discussion explicitly refers to simple shear.

2. Boundary conditions

Following Bons et al. (1997), Mandal et al. (2005) define three sets of boundary conditions (p. 1604):

(a) Homogeneous shear displacement: "The first setting can be compared with that adopted in shear box experiments, where the model is deformed in simple shear by moving plates at its four boundaries."—this is a misconception of shear boxes stemming from incorrectly designed apparatuses. As can be seen from fig. 1.1-1 of Bird et al. (2002) (theory) and from fig. 8.9a of Ghosh (1993) (apparatus), simple shear flow is driven by only two walls, the lateral walls to which the viscous matrix must adhere and not by the end walls (lateral walls of Mandal et al., 2005), which must be thoroughly lubricated and only serve to avoid collapse of the viscous matrix under its own weight (see also Marques and Coelho, 2001; Rosas et al., 2001, 2002; Bose and Marques, 2004; Marques and Bose, 2004; Marques et al., 2005). The major drawback of this approach in numerical analysis in finite element modelling (FEM) is that pressure is not explicitly constrained by the boundary settings in order to have a well-posed problem.

(b) Unconstrained lateral boundaries: "… the setting at the lateral boundaries (end boundaries in the present discussion) is given in terms of a constant pressure." Flow under these conditions is not simple shear, as shown by figs. 8a and b and 9b of Mandal et al. (2005). However, if the domain is very long and narrow, flow in its central part can approximate simple shear.

(c) Straight-out condition: "This boundary condition is comparable with that in ring shear (cf. Bons et al., 1997)."—this condition is not comparable with that of

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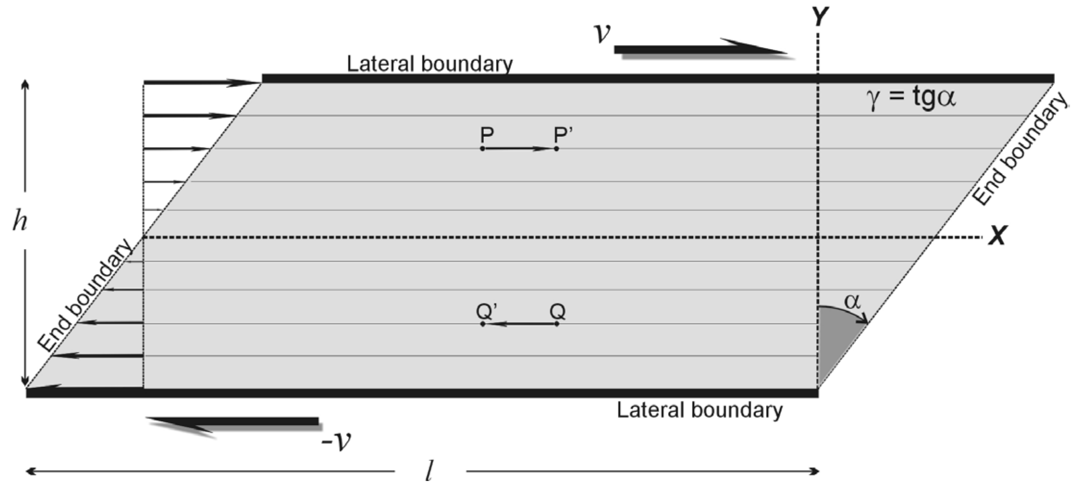

Fig. 1. Schematic representation of computational domain without inclusion. h and l are width and length of domain, respectively; v and $-v$ are velocities imposed at lateral boundaries to induce simple shear flow in the linear viscous matrix filling the computational domain; a is the angular shear strain. Shear direction is parallel to the X-axis. Black arrows at left end boundary represent the velocity profile of simple shear. P and Q are material particles displaced by simple shear flow to new positions P′ and Q′, along displacement paths represented by horizontal lines. Half arrows close to lateral boundaries indicate sense of shear.

a ring shear, because rotational Couette flow is not simple shear (dv/dh is not constant) (cf. fig. 3.6-1a of Bird et al., 2002). When the domain is large enough so that the flow near the boundaries is not affected by the rigid inclusion, the straight-out condition produces velocity profiles at the boundaries similar to the 'homogeneous shear displacement'. However, as pressure is also constrained, straight-out seems to be the best choice for simple shear conditions at the end boundaries.

3. Model parameters

The parameters defined by Mandal et al. (2005) are (1) model/inclusion dimension ratio (D_R) and (2) model aspect ratio (A_R), which seem, in principle, a correct and sensible choice. We agree with Mandal et al. (2005) that the choice of A_R is crucial for setting up a correct numerical experiment. However, a great deal of the results and discussion of Mandal et al. (2005) are based on domain ratios where the flow at end boundaries is strongly affected by the presence of the rigid inclusion, i.e. when A_R and D_R are smaller than 3–5. In such cases, setting a simple shear condition at end boundaries is incorrect and leads to erroneous results, because simple shear is not the natural solution at those boundaries, as shown by the graphs in Fig. 2. Moreover, these simulations are unrealistic, at least for geology. What is the meaning of a model shear zone with $A_R \leq 1$, as shown in all Mandal et al.'s figures from 6 to 9? What is the meaning of a square shear zone with an embedded inclusion only half, or one quarter, the size of the shear zone length, as shown in their fig. 6?

We must clarify what Marques et al. (2005) did regarding model parameters. Mandal et al. (2005) state that "In the models of Marques et al. (2005), the value of S was varied by changing both the model width and inclusion diameter but keeping the model length constant. This implies that in their analysis the model aspect ratio changed with changing S." This gives the reader the incorrect impression that Marques et al. (2005) used inappropriate values for model parameters. In the first paragraph of section 3.2, *model settings*, of Marques et al. (2005), it is clearly stated that "The length (L) was set to at least 40 times the inclusion longest axis (e_1)." Therefore, instead of keeping the model length constant, Marques et al. (2005) tried to keep the model aspect ratio always significantly greater than one (length much greater than width, as in nature), at least with a ratio that guaranteed imperceptible flow changes if model aspect ratio were increased. The statement of Mandal et al. (2005) that "It thus appears that the variation in the flow pattern that they assign only to S, perhaps includes also the effect of aspect ratio of the model." leads the reader to the incorrect conclusion that the results of Marques et al. (2005) do not depend only on S. However, Marques et al. (2005) made a sensible choice of model parameter values so that differences due to domain ratios are in the second decimal, except when D_R approaches 1. Even D_R values as small as 3–5 do not noticeably affect the position of stagnation points in the straight-out condition, despite this being the range of significant inclusion influence upon simple shear flow. On the other hand, the graph in fig. 6b of Mandal et al. (2005), which is supposed to reflect the influence of D_R, and D_R alone, on position of stagnation points, includes also the influence of S (cf. fig. 6a of Mandal et al., 2005), because the authors have kept the domain square. Therefore, their graph includes two variables, D_R and S. Otherwise it would be a straight line parallel to X, which means that the stagnation points would always be in a similar position for any given value of D_R, keeping S constant.

4. Relationship with nature

Two main characteristics of conceptual models in geology are (1) their prediction capability and (2) their relationship with natural processes. Shear zones in nature are commonly (if not always) narrow (relatively) and long, which means that their A_R must be much greater than one. Why then use model shear

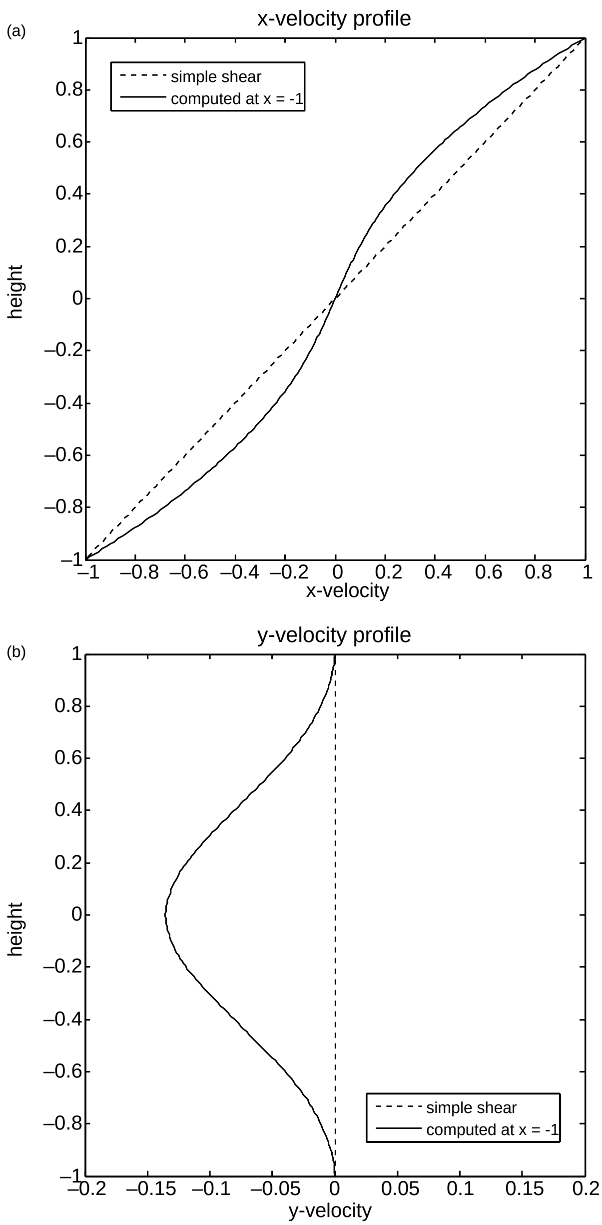

Fig. 2. Graphs of velocity profiles at end boundaries of a square domain, similar to the $D_R=2$ model in fig. 6a of Mandal et al. (2005). In the calculations, we use a circular inclusion with radius equal to 1 so that the end boundaries are at 1 and -1 for $D_R=2$. Note the great deviations of imposed simple shear velocities from the natural solution at -1 for $D_R=100$, especially regarding velocity along Y (b).

zones with A_R equal or less than one, or $D_R<5$, and why discuss them in relation to geology? One must be sensible and find an aspect ratio beyond which the results do not differ appreciably. In the past, many authors used square domains in FEM, with dimensions relatively small compared with the embedded inclusion, but that was due to computational limitations at that time.

5. Conclusions

Model dimension ratios (A_R and D_R) must have values much greater than one; preferably greater than five inclusion diameters, the region where simple shear flow is significantly disturbed by the rigid inclusion. Otherwise one imposes simple shear flow where it cannot exist, and model geometry has no relationship with nature.

The question of flow and rigid inclusion behaviour in simple shear should be restricted to finite or infinite shear zone width analysis, once it is established that the model aspect ratio should be much greater than one to be compatible with nature. What is the natural counterpart of a model shear zone with infinite width and length? The strict answer is that there is no counterpart, because infinity is a mathematical abstraction. One could argue that it is a good approximation if the natural S is much greater than one. However, this approach is not able to explain many features found in ductile shear zones, and alternative solutions must be sought. One solution seems to be, for example, confined flow. We do not agree with the conclusion of Mandal et al. (2005) that "Analytical solutions for the flow field suggest that … there cannot be any stagnation points in the flow around a rotating inclusion." It has been shown that stagnation points exist at a finite distance from the inclusion in incompressible finite shear zones. In particular, Marques et al. (2005) showed that this distance increases linearly with S. Therefore, stagnation points must also exist in infinite shear zones, but at an infinite distance to each side of the inclusion. Therefore, strictly speaking, the flow pattern should always be bow tie-shaped, although stagnation points can be positioned at infinity, in which case the pattern may seem to be eye-shaped because stagnation points are far apart and out of sight.

FEM is a very powerful tool when used with a direct relation to the natural process. Otherwise, it can produce results that are irrelevant to the deformation in rocks. We should move towards more realistic models: dynamic and three-dimensional, as opposed to the current static and two-dimensional models, instead of using parameters that do not influence a well-constrained model shear zone, which mimic deformation in rocks.

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