

# Article Paper - “Tangentially Active Polymers in Cylindrical Channels”

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This paper delves into the conformational aspects of *tangentially driven polymers* under confinement induced by the presence of walls.

**Strengths:** The field of active polymers is a growing area of research that has recently received significant attention. This paper is undoubtedly timely; until now, the effects of boundaries and confinement on active polymers, unlike their passive polymer or active point-like counterparts, have not been properly considered and understood. As someone who is passionate about this field, I found the manuscript both pleasant to read and easy to follow. The paper is logically organized into distinct sections, providing enough detail for anyone interested in reproducing the results. The findings presented here are highly encouraging because they have solid implications for the development of a more general theory for active polymers and their collective behavior. Particularly, the authors show that the effect of confinement on active polymers reveals interesting new physics that is not intuitive.

**Specific Issues, Weaknesses, and Recommendations:** I would be happy to see this paper published, but I have a few remarks - mostly minor points or requests for clarification - throughout the text and graphs that I would like to see addressed before recommending the final publication. In the following, I provide a chronological list of points (in text order) that will help the authors resolve these issues.

1. *Abstract, page 1.* “We observe that the scaling of the polymer size in the channel, quantified by the end-to-end distance, shows different anomalous behaviours at different confinement and activity conditions.” Please change “at” to “under.” Additionally, for clarity, the authors should mention that these “anomalous behaviours are compared to those of their passive counterparts.”
2. *Page 2.* Figure 1 is currently just a cosmetic cartoon. I strongly recommend that the authors introduce the relevant notation ( $F^a$  for the

polymers and the boundary conditions (such as beads and size) in the sketch.

3. *Page 2.* Can the authors comment on the role of the size of the beads in the boundary conditions? Since the characteristic size of the bead,  $\sigma$ , is chosen to be the same as for the beads in the boundary conditions, can the chain be trapped or “feel” the voids between the beads of the wall?
4. *Page 2.* Can they also provide a more in-depth explanation for the specific choice of  $\epsilon = 10, k_B T$  and  $K = 30, \epsilon$  for their simulation? They briefly mention a rather vague explanation: “This choice of parameters avoids strand crossings.” Please elaborate on the rationale behind this particular choice.
5. *Page 3, Part C.* It took me a long time to figure out what the different exponents and subscripts meant. I think it would be very helpful for any reader to *explicitly* spell out in the text what they are standing for (e.g.,  $C$  for confinement, etc.).
6. *Page 3.* In equation (10), I believe that  $\gamma$  should be read as the monomer friction coefficient  $\gamma_0$ .
7. *Page 4, Equation (17).* Please define the quantities in the text.
8. *Page 5, Figure 2.* I found the graph difficult to follow, and thus poorly convincing, at first glance, even with the help of the text. Initially, it is challenging to appreciate the significance of the changes induced by activity and for different confinements; although the different scalings are locally indicated, understanding what is interesting here proved difficult.
  - (i) I suggest that the authors first indicate the Péclet (Pe) values in (a) and (b) to guide the reader on what they are observing (essentially low activity versus high activity). I am aware that this information is provided in the caption, but the numerous variables make it hard to follow. Additionally, could they highlight the “cryptic” value  $N \simeq 200$  in this graph with a vertical line and elaborate on this critical value? Why is this value significant?
  - (ii) Since one of the main claims of the paper is that even low activity levels (as low as  $Pe = 0.03$ ) affect the conformation of the driven polymer in confinement, it is essential to show the conformation of a purely passive polymer in this graph.
9. *Page 6, figure 3),* Please also indicate the Pe values in the graph.
10. I strongly recommend that the authors add snapshots (none is shown!) of the conformation of the driven polymer in the figures when an effect is highlighted or discussed. Alternatively, they could include these snapshots as an independent figure. This addition would greatly improve reader understanding.

11. *Page 6, Figure 4.* I have the same comment as before regarding the Péclet (Pe) values. Additionally, please indicate in the caption or legend what the continuous line represents (e.g., equation 17).
12. *Page 6, Figure 5.* Could the authors comment on the non-monotonous variation of the probability density function for  $N = 750$ , low Pe?
13. *Page 7, Figure 6.* Why not use symmetry (i.e., only show half of the axis)?
14. *Page 7, Figure 7.* I appreciated the results presented here and the ensuing discussion. However, I still feel a comment on the critical value of  $N/Pe$ , at which a switch between the bulk scaling and the other scaling is observed, would be beneficial. Additionally, it would be necessary to present this graph without rescaling to appreciate the effectiveness of the proposed rescaling.
15. *Page 8, Figure 8.* For clarity, add labels such as “high confinement” in (a) and “low confinement” in (b).
  - (i) My main question pertains to the conformations here. One could show some snapshots as a function of Pe (from blue to red) which would, in my opinion, better rationalize the findings in (a).
  - (ii) Moving from low Pe values (blue) to high Pe values (red), the behavior of the chain follows the bulk behavior more closely. From the text, it is not really clear what is happening here. Higher activity generally means stiffer behavior ( $R_e$  increases) for tangentially driven chains. Does this imply that active forces are more aligned and thus the chain is propelled faster? Why would it deviate under higher confinement? What is the physical picture?
  - (iii) At low confinement (b) and low activities (0.03 & 0.05): why is there a deviation from the scaling arguments for shorter chains?
16. *Page 9* “large aspect rations”- typo - change to ratios.