Taborek Replies: In our recent Letter [1], we compared our experimentally determined contact angles with predictions of a simplified model of wetting transitions [2,3]. Detailed models of wetting [4,5] are extremely complex and are expressed in terms of many parameters which are not experimentally accessible. The simplified model achieves simplicity and utility by making some drastic approximations and assumptions, including that the solidliquid surface tension is the same as the liquid-vapor surface tension σ_{1v} and that the interaction of the fluid with the solid substrate can be described by a simple van der Waals potential. In their Comment [6], Napiórkowski and Dietrich allege that these approximations are flawed and misleading. We strongly disagree.

The only way to assess the quality of the assumptions is to compare the predictions of the model to experimental results or realistic computer simulations. This has been done for a wide variety of fluid-solid systems [2,7-11]. The results show that the simple model captures the essential physics and that it is qualitatively but not quantitatively accurate. In particular, the model generically predicts a first-order wetting transition, which is what is observed, and the functional form of the dependence of the contact angle θ with temperature is qualitatively correct. For given values of the thermodynamic properties of the fluid and a model of the fluid-solid interaction, it yields definite numerical predictions for the wetting temperature T_w and the value of $\theta(T)$ for $T < T_w$; as the cited references show, these predictions have a typical accuracy of $\pm 30\%$. The simple model also expresses the intuitively reasonable idea that the wetting temperature should be a monotonically increasing function of the room temperature contact angle.

The authors of the Comment [6] claim that the predictions of the simple model for $\theta(T)$ do not depend on the fluid-fluid interaction and cannot represent the competition that gives rise to the wetting transition and must therefore be wrong. This is a misunderstanding. The fluid-fluid interaction determines $\sigma_{lv}(T)$, and it is the temperature dependence of $\sigma_{lv}(T)$ (related to the surface entropy) that is the dominant effect that produces a wetting transition in the simple model.

The authors of Ref. [6] propose a functional form for the temperature dependence of the contact angle of water on graphite which describes our data rather well. Unfortunately, the physical motivation for the functional form and the relationship between the numerical parameters that it contains to the model described in the Comment is not clear. Hopefully, the authors will explain the relationship in more detail in a future publication.

Because of its successful track record, the simple model has been used as a benchmark of comparison in most recent studies focused on analysis of data from real or computer simulations of wetting transitions. Like other zeroth-order models (e.g., the Drude model and the van der Waals equation of state), it provides a framework to understand a wide range of data, and deviations of the model predictions from the data provide useful hints about new physics; the failure of the simple model to account for the behavior of $\theta(T)$ on substrates with low values of the room temperature contact angle may be an example of this. To criticize the simple model for the crudeness of its approximations is to miss the point of its utility. A perhaps more interesting question is, despite the crudeness of the approximations, why does it usually work so well? Finally, it is important to note that the basic experimental results of our Letter do not depend on the accuracy of the simple model or any other model.

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- S. R. Friedman, M. Khalil, and P. Taborek, Phys. Rev. Lett. 111, 226101 (2013).
- [2] E. Cheng, M. W. Cole, W. F. Saam, and J. Treiner, Phys. Rev. B 48, 18214 (1993).
- [3] S. Gatica and M. Cole, J. Low Temp. Phys. 157, 111 (2009).
- [4] A. O. Parry and C. J. Boulter, Physica (Amsterdam) 218A, 77 (1995).
- [5] S. Dietrich and M. Napiórkowski, Phys. Rev. A 43, 1861 (1991).
- [6] M. Napiórkowski and S. Dietrich, preceding Comment, Phys. Rev. Lett. 114, 039601 (2015).
- [7] R. Garcia, K. Osborne, and E. Subashi, J. Phys. Chem. B 112, 8114 (2008).
- [8] F. Ancilotto and F. Toigo, Phys. Rev. B 60, 9019 (1999).
- [9] M. S. Sellers and J. R. Errington, J. Phys. Chem. C 112, 12905 (2008).
- [10] W. Shi, J. K. Johnson, and M. W. Cole, Phys. Rev. B 68, 125401 (2003).
- [11] X. C. Zhao, Phys. Rev. B 76, 041402(R) (2007).