

Thermal conductivity of composites: How Comsol revealed an omission in a classical paper

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Initial objective: Develop and validate a method for the prediction of the equivalent thermal conductivity T_0 of a particulate composite.

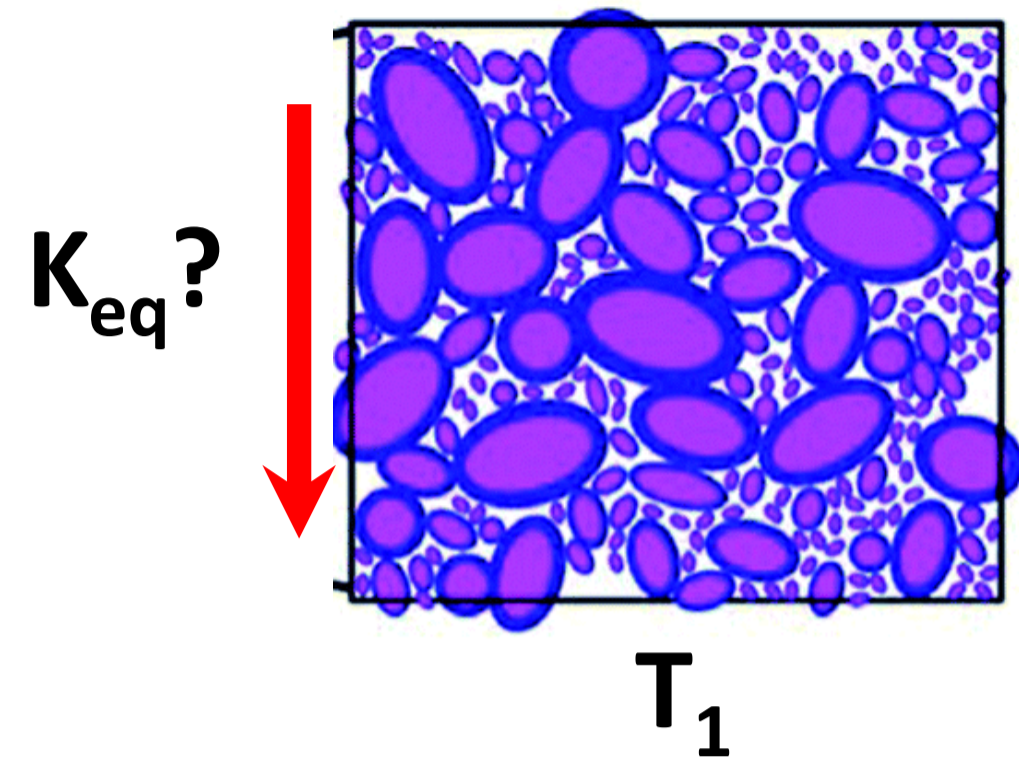


Figure 1. The problem to be solved

Revisiting Nan's model: Based on the calculation of the equivalent conductivity of a particle + resistive layer

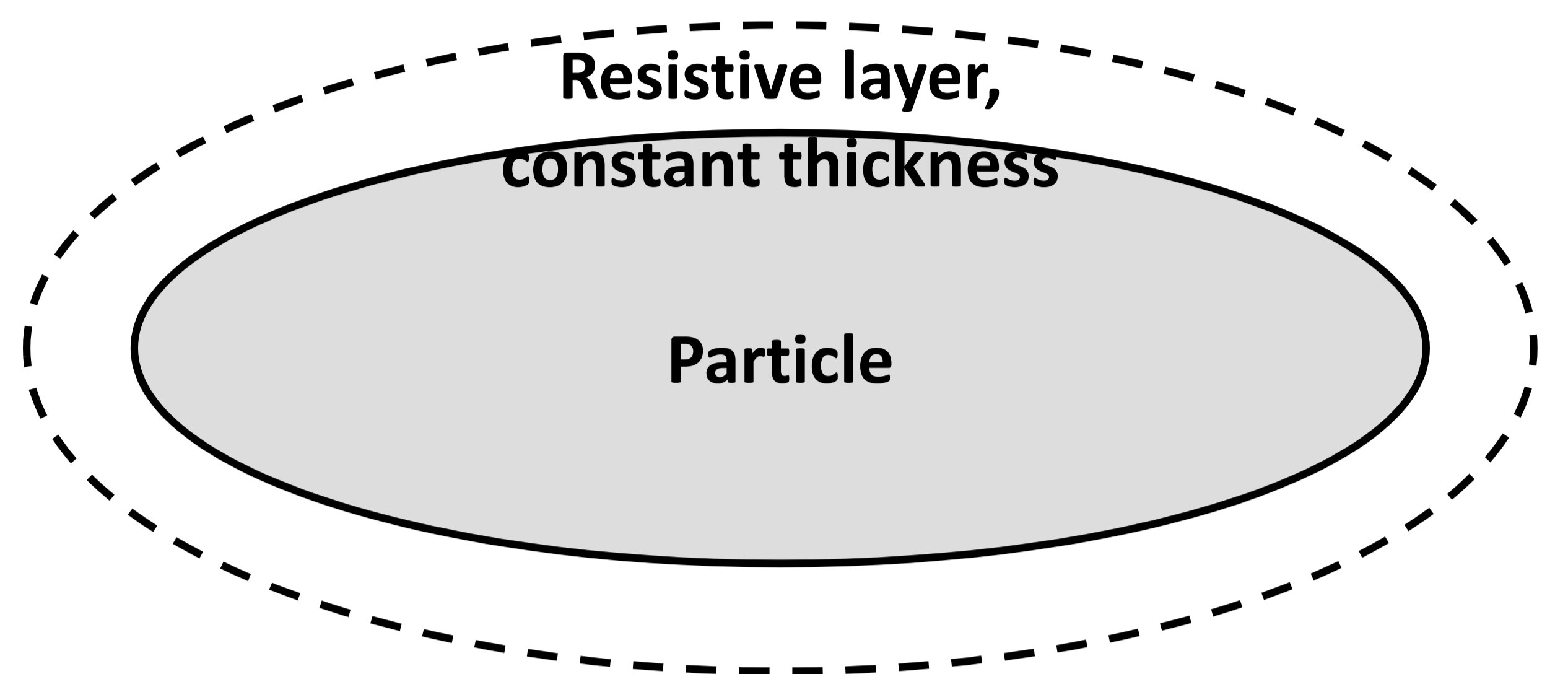


Figure 5. Particle + resistive layer

A simple procedure with Comsol:

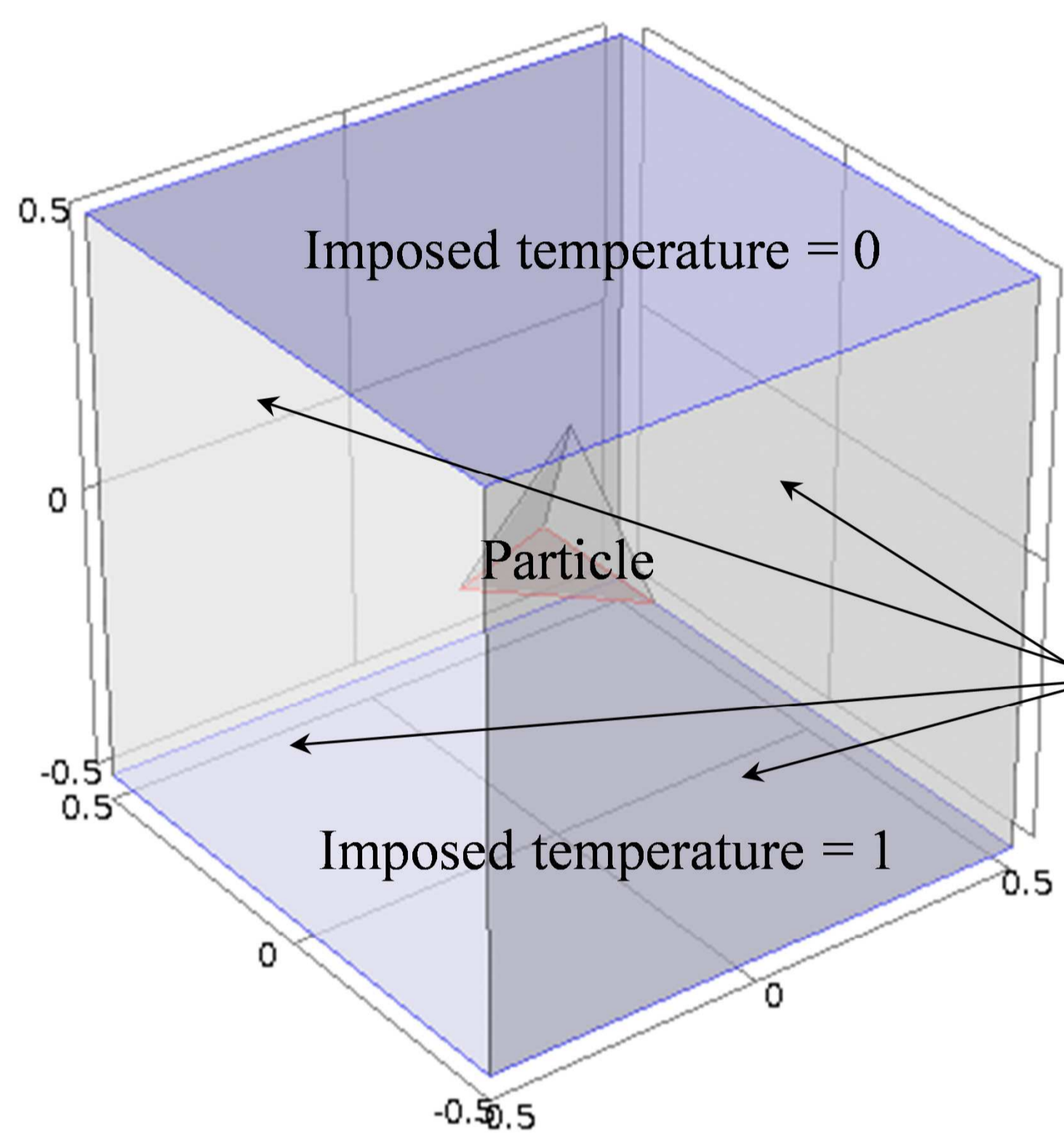


Figure 2. Domain and boundary conditions

Inside the domain:

$$\nabla \cdot (K_i \nabla T_i) = 0$$

At the particle/matrix interface:

$$-K_m \frac{\partial T_m}{\partial n_m} = \frac{T_m - T_p}{R_{Bd}} = K_p \frac{\partial T_p}{\partial n_p}$$

Interfacial resistance

Implicit assumptions:

- resistive layer is also an ellipsoid
- has same aspect ratio as the particle

=> **False in the general case**

=> **Two contributions must be added !**

Aspect ratio contribution could be included in revised model, **much improved match:**

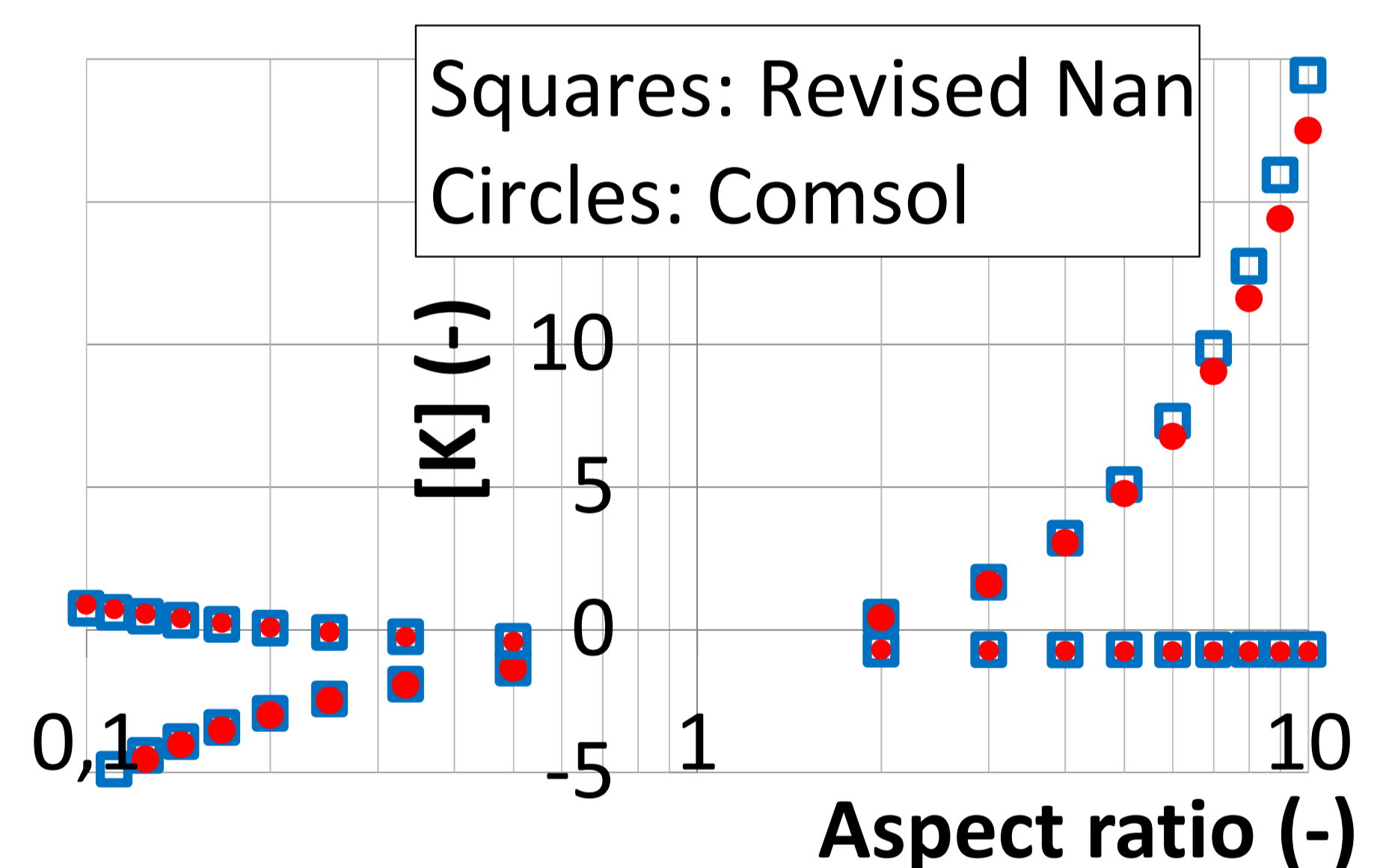


Figure 6. Ellipsoids, revised model

Validation against a popular model: Nan et al. [1], ellipsoidal particles. Almost 600 cites !

Figure 3. Spheres

Good match for spheres

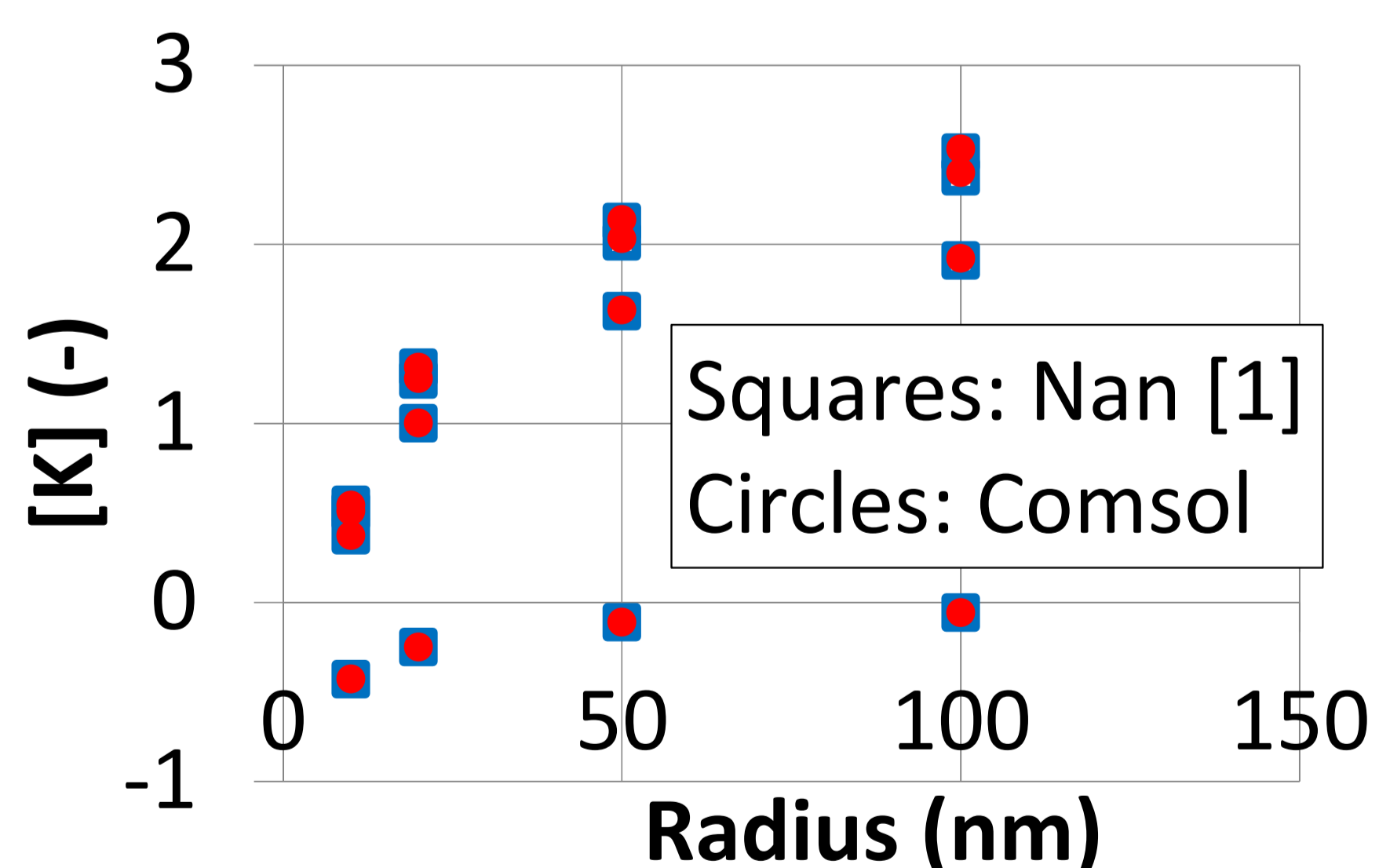
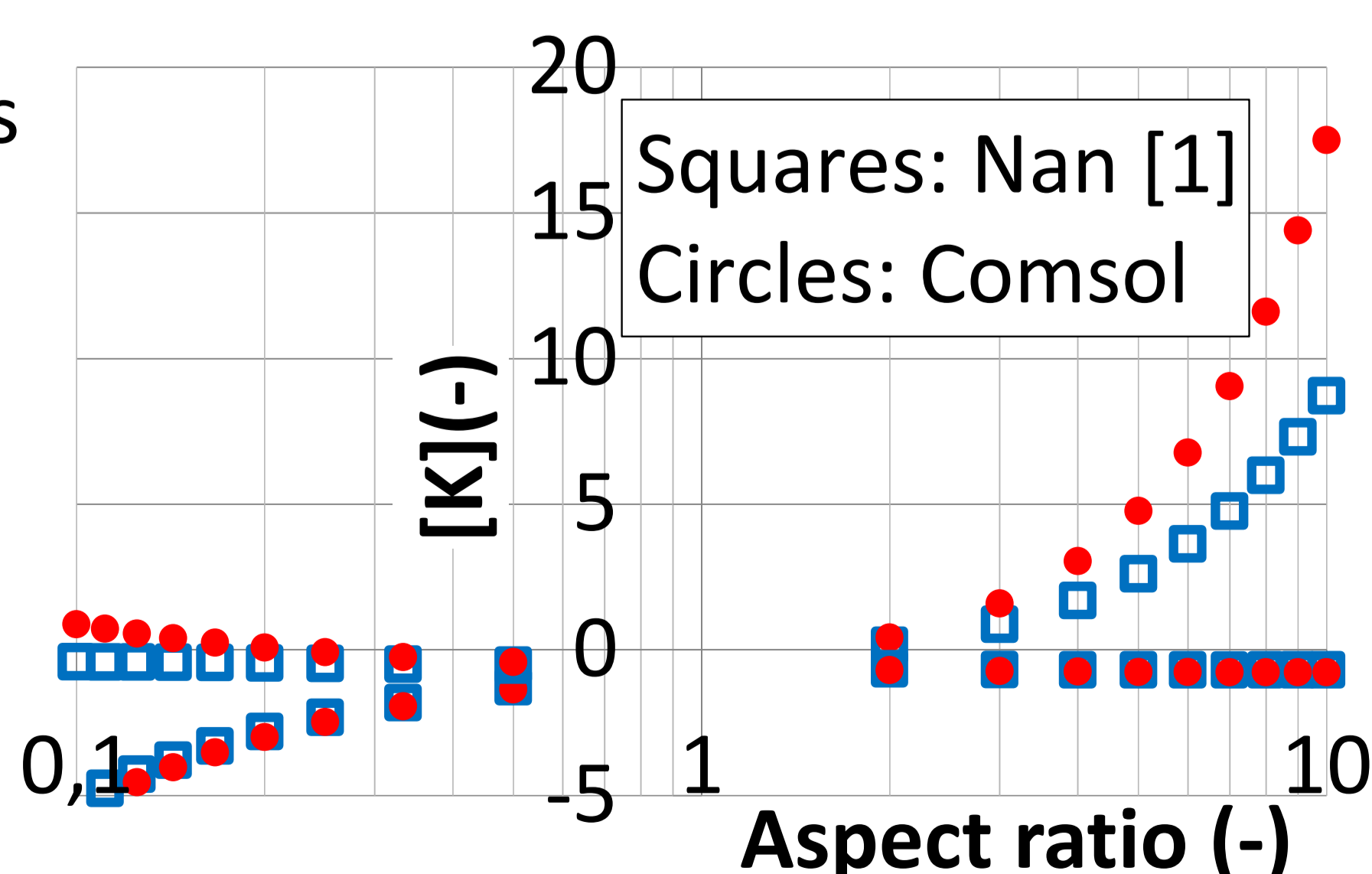


Figure 4. Ellipsoids

Very poor for ellipsoids



Conclusions: An improved model is established, satisfying from theoretical point of view. Practical consequences are thought to be minimal.

References:

1. Nan C.W., Birringer R., Clarke D.R. and Gleiter H., Effective thermal conductivity of particulate composites with interfacial thermal resistance, *Journal of Applied Physics*, **81**, 10, 6692-6699 (1997)