

Are they answering the question?

"Although no evaporation of guaiacol from the interface into the gasphase could be observed during the time-frame of simulation (50 ns) it is reasonable to assume that the increase in the probability of finding guaiacol at the interface leads to a higher probability of its evaporation."

If you want to study evaporation, study evaporation!

(Anyone know any tricks to extend the timescale accessible to a simulation?)