

Figure 1: Dependence of the pressure P applied to the gel in order to compress it to a certain density as a function of this gel density  $\varphi$  for different (a) ionization constant pK of the gel, (b)-(c) solvent quality and (d)-(e) salt concentration  $c_s$ .

## 2.3.2. Box-model predictions

(VP.27.4) Do we need to add these plots as our expectation from MD based? If yes, I'll improve pictures, If not then I'll just delete them

Eq. 7 can provide us a set of pressure-extension curves varying, e. g. salt concentration. Afterwards we can convert this set into a phase diagram, e. g. in coordinates of salt concentration - gel density as shown in Fig. 5. In Fig. 5(a) we plot several phase diagram for different solvent quality at constant pH - pK = 2, while in Fig. 5(b) we show how pH - pK difference change the phase diagram. Each of them has a U-shaped curvature. Firstly, an increase of pH - pK difference that can be considered as an increase of pH or moving to more charged PE gel leads to the presence of hydrogel in two phases states at lower salinity. Secondly, a deterioration of the solvent quality (increase  $\chi$ ) results in a shift of the curves to high salt concentrations, thereby increases the region of two phases states of the hydrogel. Thus, we expected from simulations similar results.