# The Interface Width of Separated Two-Component Lipid Membranes

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We study two-component vesicles with coherent domains of the components, where the domains are separated by an interface. The components are characterized by different spontaneous curvatures. No line tension term or interactions between components are included in the model. The influence of the interface width and interface location on the bending energy and shape of the vesicles is studied. How the spontaneous curvature of one component influences the concentration profile is examined. The vesicles of oblate and prolate geometries are investigated.

#### Introduction

Lipid membranes are models of two-dimensional fluids. The bilayer membrane forms a surface embedded in threedimensional space. Multicomponent membranes compared to one-component membranes have extra degrees of freedom associated with the distribution of components within the membrane. The distribution of membrane components influences the shape of the membrane, but it is also possible that the shape of the membrane may influence the distribution of the components.<sup>1-4</sup> Such mutual dependence of membrane shape and distribution of components may lead to many interesting physical phenomena which are important for functioning biological systems. One may speculate that the change of membrane shape may lead to the separation or mixing of membrane components. It may also be possible that, due to minimization of the curvature energy, the components which are separated in a flat membrane may be mixed in a curved membrane which forms the vesicle (and vice versa).

Biological membranes are built from many components such as lipids, proteins, and polymers. It may happen that the membrane constituents phase separate and two liquid phases coexist in the membrane. 2,3,5-7 The coexisting liquid phases are separated by an interface. The formation of domains in lipid membranes and influence on the membrane shape have been the subject of many studies.<sup>8-11</sup> The formation of ordered domains and budding of domains were of particular interest. Membranes and vesicles with domains separated by the interface with zero width have been studied previously within the framework of the curvature energy model. 12-21 In the strong segregation limit which implies the interface of zero width, the shape transitions of domains have been observed. 16-18 It has been predicted that the change of the domain size induces the shape transformation of membranes. 16-19 Here, we would like to investigate the influence of the geometry of a vesicle on the separation of the components. The driving force for the separation is the compatibility of the local curvature of a vesicle to the spontaneous curvatures of components. We concentrate on the interface between the domains and study the mutual dependence of the vesicle shape and the thickness of the interface. The problem is studied within the framework of the curvature energy model.<sup>22-24</sup> It is assumed that the mixture is in the state of vanishing line tension.

#### 2. Model and Parametrization

The components are characterized by the spontaneous curvatures  $\mathcal{C}_0^A$  and  $\mathcal{C}_0^B$ . It means that, if the membrane is built from one component, the optimal shape which minimizes the bending energy is the surface of constant mean curvature equal to the spontaneous curvature of that component. This is an ideal situation which almost never happens in real systems because of the constraints imposed on the topology, volume, and surface area of the vesicles. These constraints are the result of a specific physical situation. We investigate the simplest case of vesicles with spherical topology. It is assumed that the components are separated and form coherent domains. The spontaneous curvature of one component is zero, and the spontaneous curvature of the other one is positive. The model may also describe the situation in which some molecules are attached to the membrane and form coherent regions. In that case, the attached molecules impose the spontaneous curvature on the membrane.<sup>25–28</sup>

The energy of the studied system depends on the curvatures of the membrane. It is the sum of the integrals from the mean curvature and the Gaussian curvature over the surface of a vesicle. $^{22-24}$ 

$$\mathcal{F} = \frac{\kappa}{2} \int_{S} dS (\mathcal{C}_{1} + \mathcal{C}_{2} - \mathcal{C}_{0})^{2} + \bar{\kappa} \int_{S} dS \mathcal{C}_{1} \mathcal{C}_{2}$$
 (1)

where  $\kappa$  and  $\bar{\kappa}$  are the bending and Gaussian rigidity,  $\mathcal{C}_1$  and  $\mathcal{C}_2$  are the principal curvatures,  $\mathcal{C}_0$  is the spontaneous curvature, and the integral (eq 1) is taken over the surface of a closed vesicle. The first integral describes elastic properties of a membrane. The second integral describes topological changes.

It is assumed for simplicity that the bending rigidity and the Gaussian rigidity are the same for both components.

$$\bar{\kappa} = \bar{\kappa}^{A} = \bar{\kappa}^{B} \tag{2}$$

$$\kappa = \kappa^{A} = \kappa^{B} \tag{3}$$

Since there is no difference between the Gaussian rigidity of the two components and no topological changes are allowed, the integral from the Gaussian curvature contributes a constant value and is not taken into the calculations. We investigate the limit of large bending rigidity. Thus, the entropy of mixing is small compared to the curvature energy and is neglected in the calculations. We consider vesicles which have rotational symmetry and the mirror symmetry with respect to the equator of the vesicle. Thus, the domains are distributed symmetrically in such a way that the domains of one component are located at the poles of the vesicle and are separated by the domain of the other component located along the equator. The vesicle profile is parametrized with the angle,  $\theta$ , of the tangent to the profile with the symmetry plain as a function of the arclength, s. The surface of a vesicle in 3D Euclidean space is described by the following equations:

$$z(s) = \int_0^s ds' \sin[\theta(s')]$$
 (4)

$$x(s, \psi) = r(s)\cos(\psi) \tag{5}$$

$$y(s, \psi) = r(s)\sin(\psi) \tag{6}$$

where  $\psi$  is a rotation angle and r(s) is the radius, given by the following equation

$$r(s) = \int_0^s ds' \cos[\theta(s')]$$
 (7)

The following boundary conditions must be satisfied for vesicles which have mirror symmetry with respect to the equator of the vesicle.

$$\theta(0) = 0 \tag{8}$$

$$\theta(L_{s}/2) = \pi/2 \tag{9}$$

where  $L_s$  is the length of the shape profile. The bending energy for parametrization of a vesicle with the function  $\theta(s)$  is given by the following formula.

$$\mathcal{F}[\theta(s), \phi(s)] = \frac{\kappa}{2} \int_0^{2\pi} d\psi \int_0^{L_{s/2}} ds r(s) \left[ \frac{d\theta(s)}{ds} + \frac{\sin(\theta(s))}{r(s)} - \mathcal{G}_0(\phi(s)) \right]^2$$
(10)

 $\psi$  is the angle of rotation, and  $\phi(s)$  is the concentration profile. The functional depends on two functions which describe the concentration profile and the shape of the vesicle. It has to be noted that  $\theta(s)$  and  $\phi(s)$  are not arbitrary functions. Some restrictions, resulting from the physical situation, are imposed on the form of the function which minimize the functional.

We consider concentration profiles which have the form of the hyperbolic tangent given by the following equation.

$$\phi(s) = \pm \frac{1}{2} [\tanh(\xi(s - s_0)) + 1]$$
 (11)

 $\xi$  describes the interface width, and  $s_0$  defines the location of the interface. In eq 11, plus sign (+) is used when the concentration is larger at the equator and minus (-) sign when the concentration is larger at the poles of the vesicle. The hyperbolic tangent is often used to model an interface profile of simple phase-separated bulk mixtures. Therefore, it may be expected that the choice of the hyperbolic tangent for phase-separated lipid membranes will also be a reasonable approximation. The function describing the interface profile, given by eq 11, depends only on two parameters  $\xi$  and  $s_0$ . The location of the interface is mostly determined by the constraint on the total concentration  $\phi_{\text{tot}}$ , which can be calculated from the concentration profile as the following integral over the surface of a vesicle:

$$\phi_{\text{tot}} = \int_0^{2\pi} \psi \int_0^{L_s/2} ds r(s) \phi(s) / S$$
 (12)

where S is the surface area of the vesicle given by eq 14.

The membrane shape may influence the distribution of the components in the membrane, which can lead to the segregation of components. On the other hand, the distribution of the components determines the membrane shape. These two processes are coupled in some complex way. It is our intention to study this coupling in a very simple model where we will be able to analyze in detail different aspects of this coupling. In the present study, the coupling is implemented in a simple way. The spontaneous curvature is coupled to the concentration.

$$\mathcal{C}_0(s) = \phi(s)(\mathcal{C}_0^A - \mathcal{C}_0^B) + \mathcal{C}_0^B$$
 (13)

 $\mathcal{C}_0^A$  and  $\mathcal{C}_0^B$  are the spontaneous curvatures of the membrane occupied by the first and second components, respectively. The coupling of the spontaneous curvature to the concentration introduces the dependence of the distribution of components on the shape of a vesicle. We would like to examine the shape of the optimal concentration profile which minimizes the bending energy. Especially, we are interested in the interface width and its dependence on the value of the spontaneous curvature

The experimental conditions we would like to mimic are such that the surface area S and the volume V of the vesicle are constant. The surface area and the volume are calculated from the following formulas.

$$S = 2\pi \int_0^{L_s/2} \mathrm{d}s r(s) \tag{14}$$

$$V = \pi \int_0^{L_s/2} \mathrm{d}s r^2(s) \sin\theta(s) \tag{15}$$

The radius,  $R_0$ , and the volume,  $V_0$ , of the sphere which has the same surface area as the studied vesicle are chosen as the units of length and volume, respectively.  $R_0$  and  $V_0$  are used to define the reduced volume and dimensionless spontaneous curvatures

$$v = V/V_0 \tag{16}$$

$$c_0^{\alpha} = \mathcal{G}_0^{\alpha} R_0 \tag{17}$$

where  $\alpha$  stands for components A or B. The control parameters for the studied process are the reduced volume, total concentration,  $\phi_{\text{tot}}$ , and the spontaneous curvatures  $\mathcal{C}_0^{\alpha}$ .

If we assume that the optimal state of the membrane is the state with the minimal bending energy, then there is some particular shape and particular distribution of components which minimize the bending energy. The functional (eq 10) is minimized numerically. The function  $\theta(s)$  is expressed as a Fourier series

$$\theta(s) = \theta_0 \frac{2s}{L_s} + \sum_{i=1}^{N} a_i \sin\left(\frac{2\pi}{L_s} i \cdot s\right)$$
 (18)

where N is the number of the Fourier modes, and  $a_i$  are the Fourier amplitudes.  $\theta_0$  is the angle at the equator of the vesicle,  $\theta_0 = \pi/2$ . When the function  $\theta(s)$ , in the form of the Fourier series given by eq 18, is plugged into eqs 7, 4, and 10, the functional minimization can be replaced by the minimization of the function of many variables. The functional (eq 10) becomes the function of many variables, which are the amplitudes  $a_i$  and the length of the shape profile  $L_s$ . Since the

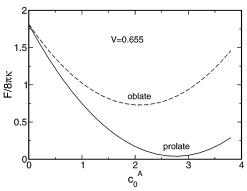
functional is minimized with respect to the shape and concentration profile, two additional variables  $\xi$  and  $s_0$ , which determine the concentration profile, are also used in the minimization. The minimization is performed under the constraints of constant surface area S and volume V. The constraints in numerical calculations are implemented with the help of Lagrange multipliers.

### **Results**

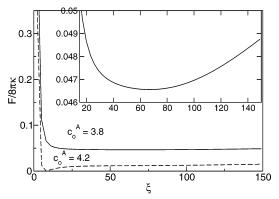
The aim of this work is to examine the influence of the concentration profile on the elastic energy and the shape of a vesicle. The specific feature of the present study is the coupling of the concentration profile to the shape of the vesicle via the spontaneous curvature. From the concentration profile, which results from the minimization of the functional (eq 10), we obtain information about the interface width for two different geometries of vesicles (oblate and prolate). We consider the situation where the composition of the membrane is constant. The location and the width of the interface are examined for a few concentrations of the components  $\phi_{tot}$ . The spontaneous curvature of the membrane components are used as material parameters. By varying the spontaneous curvature, we can model the properties of the componets which form the membrane. We investigate the situation where the membrane does not stretch. Thus, the surface area and the volume do not change. The reduced volume v is chosen is such a way to obtain, for onecomponent membranes with the spontaneous curvature equal to 0, solutions with different geometries (oblate, prolate).

We have examined one-component vesicles with different spontaneous curvatures as a prerequisite to the study of twocomponent vesicles. When we assume that the total surface of the membrane is occupied by one component, the function which describes the composition of the membrane is constant  $\phi(s) =$ 1.0. For a range of reduced volume close to v = 0.65 and the spontaneous curvature equal to zero,  $c_0^{\rm A} = 0$ , there exist two solutions of the bending energy functional, for oblate and prolate vesicles.<sup>29</sup> Which solution is stable depends on the value of the reduced volume. The reduced volume for which prolate and oblate families of shapes have the same energy is estimated as v = 0.65. For the reduced volume larger than v = 0.65, prolate vesicles are the stable solution, and for the reduced volume smaller than v = 0.65, oblate vesicles are the stable solution. The reduced volume of all vesicles studied in this paper is chosen to be v = 0.655. Since we are going to study the vesicles built of two components that have different spontaneous curvatures, we calculated the energy for two branches of prolate and oblate shapes with nonzero spontaneous curvatures in order to determine which spontaneous curvature is optimal for the reduced volume of 0.655. For the reduced volume v = 0.655and the uniform distribution of the spontaneous curvature, the vesicles with the prolate geometry are more stable than the vesicles with oblate geometry. The optimal spontaneous curvature for the branch of oblate vesicles is in the vicinity of  $c_0^A$ = 2 and for the branch of prolate vesicles in the vicinity of  $c_0^A$ = 2.8, as shown in Figure 1. Thus, it may be expected that the increase of the spontaneous curvature even on some region of the vesicle will lower its bending energy.

We study the vesicles of oblate and prolate geometry, with domains of nonzero spontaneous curvature. The geometry of the vesicle influences the distribution of the components due to the coupling of the spontaneous curvature with the concentration profile. It is easy to distinguish in oblate vesicles two regions where the local mean curvature is small and where the local curvature is large. In the vicinity of the poles, the local



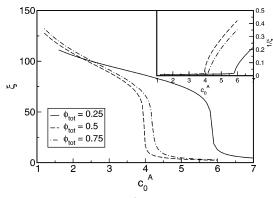
**Figure 1.** The bending energy for one-component vesicles at the reduced volume v = 0.655 as a function of the spontaneous curvature. Oblate vesicles, dashed line; prolate vesicles, solid line. The function which describes concentration profile has a simple form  $\phi(s) = 1.0$ .



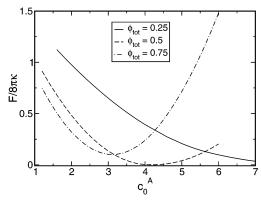
**Figure 2.** The bending energy as a function of the parameter  $\xi$  for oblate vesicles. The reduced volume v=0.655. The spontaneous curvature  $c_0^A=3.8$  is represented by the solid line and  $c_0^A=4.2$  the dashed line. The total concentration  $\phi_{\rm tot}=0.5$ . The inset shows the magnification of the curve for the spontaneous curvature  $c_0^A=3.8$ .

mean curvature is small, while in the vicinity of the equator, the local curvature is much larger. Thus, to minimize the bending energy, the components with larger spontaneous curvature will occupy the region of the vesicle at the equator, and the components with smaller spontaneous curvature will occupy the poles of the vesicle. We study the size of the interface width, at constant total concentration  $\phi_{\text{tot}}$ , as a function of the spontaneous curvature of one component,  $c_0^A$ , keeping the spontaneous curvature of the other component equal to zero,  $c_0^{\rm B} = 0$ . The interface width described by the parameter  $\xi$  and the interface position  $s_0$  are calculated during the minimization of the functional (eq 10). The location of the interface  $s_0$  is determined mostly by the constraint imposed on the total concentration of components. The size of the interface width gives an indication of the tendency for separation of the components within the membrane. When the interface width is small ( $\xi$  is large), one may expect that the membrane components prefer to be separated, and widening the interface indicates the tendency for mixing.

We have examined how the bending energy depends on the parameter  $\xi$  which determines the interface width. The functional (eq 10) was minimized with  $\xi$  kept as a parameter, for an oblate vesicle with the reduced volume v=0.655, the total concentration  $\phi_{\rm tot}=0.50$ , and a few values of the spontaneous curvature. Figure 2 shows the bending energy resulting from the minimization of the functional (eq 10) as a function of the parameter  $\xi$  for two values of the spontaneous curvature  $c_0^{\rm A}=3.8$  and  $c_0^{\rm A}=4.2$ . There is a value of the interface width for which the bending energy has a minimum. For  $c_0^{\rm A}=4.2$ , the minimum is deep



**Figure 3.** The interface width  $\xi$  as a function of the spontaneous curvature  $c_0^{\rm A}$  for oblate vesicles for the reduced volume v=0.655. The lines represent the interface width for three values of the total concentration  $\phi_{\rm tot}=0.25$  (solid line),  $\phi_{\rm tot}=0.50$  (dashed line), and  $\phi_{\rm tot}=0.75$  (dashed—dotted). In the inset, the inverse of  $\xi$  is plotted.



**Figure 4.** The bending energy as a function of the spontaneous curvature  $c_0^A$  for oblate vesicles for the reduced volume v=0.655. The lines represent the interface width for three values of the total concentration  $\phi_{\text{tot}}=0.25$ ,  $\phi_{\text{tot}}=0.50$ , and  $\phi_{\text{tot}}=0.75$ .

and is located for small values of  $\xi$  which indicates a wide interface. For  $c_0^A=3.8$ , the minimum is shallow and is located for large values of  $\xi$  which indicates a sharp interface. The shallow minimum is presented in the inset of the Figure 2. Since the minimum is shallow, it may be expected that the interface width can undergo significant fluctuations. However, the interface width should remain narrow during those fluctuations. Varying the spontaneous curvature  $c_0^A$ , one may expect the existence of the transition from the systems with a narrow interface to a wide interface. It is interesting to know what is the nature of that transition, whether that transition is continuous or discontinuous.

We have examined how the interface width of the concentration profile depends on the spontaneous curvatures of one component  $c_0^A$ . The spontaneous curvature of the other component was kept constant  $c_0^{\rm B}=0$ . Figures 3 and 4 show the interface width and the bending energy as a function of the spontaneous curvature  $c_0^A$ . The functional (eq 10) was minimized at the reduced volume v = 0.655 for an oblate vesicle and for three values of the total concentration  $\phi_{\text{tot}} = 0.25$ ,  $\phi_{\text{tot}}$ = 0.5, and  $\phi_{tot}$  = 0.75. The functional (eq 10) was minimized for each value of the spontaneous curvature,  $c_0^A$ , and the curves shown in Figures 3 and 4 represent the values of the variable  $\xi$ and the bending energy obtained from the minimization of the functional. It can be seen from Figure 3 that the shapes of the curves which represent the bending energy as a function of  $\xi$ are similar for all three values of the total concentration  $\phi_{\text{tot}}$ . When the spontaneous curvatures  $c_0^A$  is small, the optimal

value of  $\xi$  is high and the interface width is narrow. When the spontaneous curvature  $c_0^{\rm A}$  becomes larger, the value of  $\xi$  decreases smoothly, initially slowly and at some value of  $c_0^{\rm A}$ rapidly. Two regimes can be distinguished: high  $\xi$  regime/ narrow interface and small  $\xi$  regime/wide interface. It can be interpreted as the regimes of well-separated and partially mixed membrane components. The particular value of the spontaneous curvature  $c_0^A$ , for which the transition from the first regime to the second regime occurs, depends on the geometry of the vesicle and the location of the interface  $s_0$  which determines how much of the vesicle surface is occupied by the component with the higher spontaneous curvature  $c_0^A$ . One can speculate that, if the spontaneous curvatures of the membrane components differ substantially, then the components tend to be mixed in order to minimize the bending energy. Thus, mixing components which have significantly different spontaneous curvatures should be avoided in order to prepare vesicles with well-defined domains.

The distribution of components in the membrane alters the shape of the membrane and the bending energy. The bending energy presented in Figure 4 changes smoothly with the change of the spontaneous curvature  $c_0^A$  and does not decrease or increase substantially in the region of the rapid change of the parameter  $\xi$ . Since the bending energy depends on the shape of the vesicle, any significant change of the vesicle shape should not be expected. The vesicle shape changes smoothly with the change of the spontaneous curvature  $c_0^A$ . Figure 5 shows two sets of vesicle shapes for two values of the total concentration  $\phi_{\text{tot}} = 0.50$  (Figure 5a,b,c) and  $\phi_{\text{tot}} = 0.25$  (Figure 5d,e,f). Three shape profiles are chosen for each value of the total concentration  $\phi_{tot}$ . The first profile is chosen for small values of the spontaneous curvature, large values of  $\xi$  (Figure 5a,d). The second profile is chosen for the values of the spontaneous curvature just before the rapid change of  $\xi$ , where  $\xi$  is still large (Figure 5b,e). The third profile is chosen for the values of the spontaneous curvature just after the rapid change of  $\xi$ , where  $\xi$ is small (Figure 5c,f). The shape changes smoothly from concave to convex, in the region of large values of the variable  $\xi$ , and is due to the change of the spontaneous curvature  $c_0^A$ , since the interface width remains narrow. The second and third profiles are very similar, despite a large change of the interface width. Thus, the change of the interface width is not significantly reflected in the shape of the vesicle. However, it is favorable for the bending energy to have a wide (smooth) interface instead of a narrow (sharp) interface when the difference between the spontaneous curvature of the membrane components is large. The jump of the spontaneous curvature at a very sharp interface may be unfavorable for minimizing the bending energy, when the difference of the spontaneous curvatures is large. The bending energy may be minimized in such a case by widening the interface between the domains. In the strong segregation limit, where the interface is narrow due to the highly unfavorable interactions between unlike components, the minimization of the bending energy may cause widening of the interface if the gain in the bending energy is sufficiently big to compensate the energy lost by the increase of the area of contact between the unlike components. The other possibility is shrinking of the interface line at the expense of the bending energy, which may lead to budding of a vesicle.

Figure 6 shows the sum of the principal curvatures  $c_1(s) + c_2(s)$  and the local spontaneous curvature  $c_0(s)$  which is a function of the concentration profile  $\phi(s)$ . The curvature profiles shown in Figure 6 correspond to the shape profiles presented in Figure 5. The curves shown in Figure 6 by the dashed line

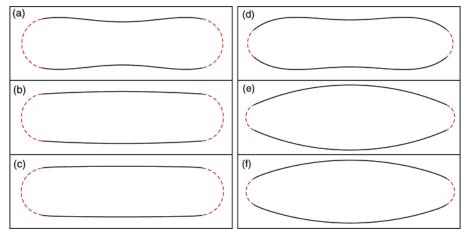


Figure 5. The shape profiles for oblate vesicles with the reduced volume v = 0.655. The dashed lines and the solid lines represent the region of the vesicle occupied by the components with positive spontaneous curvature  $c_0^A$ , and  $c_0^B = 0.0$ , respectively. The lines meet at the inflection point of the hyperbolic tangent  $s_0$ . On the left, the profiles are presented for the total concentration  $\phi_{\text{tot}} = 0.5$  and for the spontaneous curvature (a)  $c_0^A = 2.00$ , (b)  $c_0^A = 3.96$ , and (c)  $c_0^A = 4.12$ . On the right, the profiles are presented the total concentration  $\phi_{\text{tot}} = 0.25$  and for the spontaneous curvature (d)  $c_0^A = 2.60$ , (e)  $c_0^A = 5.8$ , and (f)  $c_0^A = 6.10$ .

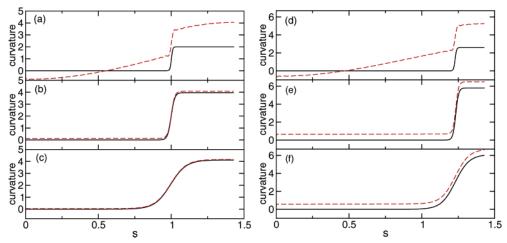


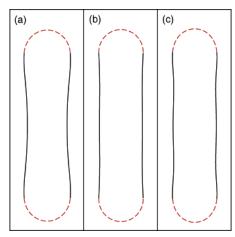
Figure 6. The spontaneous curvature profiles  $c_0(s)$  (solid lines) and the local curvature  $c_1(s)+c_2(s)$  (dashed lines) for oblate vesicles at the reduced volume v=0.655. s is the arclength. The profiles presented here start at the pole of the vesicles s=0 and end at the equator of the vesicles  $s=L_s/2$ . On the left, the profiles are presented for the total concentration  $\phi_{\text{tot}}=0.5$  and for the spontaneous curvature (a)  $c_0^A=2.00$ , (b)  $c_0^A=3.96$ , and (c)  $c_0^A=4.12$ . On the right, the profiles are presented for the total concentration  $\phi_{\text{tot}}=0.25$  and for the spontaneous curvature (d)  $c_0^A=2.60$ , (e)  $c_0^A=5.80$ , and (f)  $c_0^A=6.10$ .

represent the functions which minimize the functional (eq 10). The functions are not arbitrary; one should remember about the constraints imposed on the shape of those function. It is interesting to note that the optimal value of the bending energy is obtained when the curve which describes the local curvature is parallel to the curve which describes the spontaneous curvature profile and is the lowest when they overlap. The concentration profiles studied in this paper describe two domains of different spontaneous curvatures separated by an interface. Figure 6a,b,d,e shows the profile with a sharp interface between the domains. Figure 6c,f shows the profiles with a wide interface between the domains. The difference between the spontaneous curvature profile and the curvature profile is almost invisible in the Figure 6c. This leads to very small values of the bending energy, which is almost zero. The change of the interface width from sharp to wide is not reflected significantly in the shape of the vesicles and therefore in the bending energy.

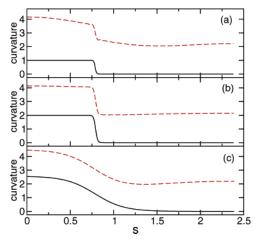
The overall behavior remains similar when the geometry of the vesicles is changed from oblate to prolate. However, for prolate vesicles, the distribution of components  $\phi(s)$ , and therefore the distribution of the spontaneous curvatures  $c_0(s)$ , cannot be so easily matched to the local curvatures because of

the constraints imposed on the shape of the vesicle. Figures 7 and 8 show the shape profiles and the curvature profiles for the prolate vesicles at the reduced volume v=0.655 and the total concentration  $\phi_{\rm tot}=0.25$ . The curvature profiles shown in Figure 8 correspond to the shape profiles presented in Figure 7. The distribution of components for prolate vesicles differ from the distribution of components for oblate vesicles. Unlike in the case of oblate vesicles, in the prolate vesicles, the component with positive spontaneous curvature is located at the poles of the vesicle and the component with  $c_0^{\rm B}=0.0$  is distributed at the equator of the vesicles. The distribution of the components results from the geometry of the prolate vesicle. The local curvature at the equator is smaller than the local curvature at the poles of the vesicle.

The conclusions obtained for the oblate vesicles apply also to the prolate ones. Similarly as for oblate vesicles, it is possible to distinguish two regions of wide and narrow interfaces and transition between those regions. Each region is characterized by sharp and wide interfaces as shown in Figure 8a,b and Figure 8c, respectively. The change of the shape with the change of the spontaneous curvature  $c_0^{\rm A}$  is not significant. The energy is a



**Figure 7.** The shape profiles for prolate vesicles with the reduced volume v = 0.655. The dashed lines and the solid lines represent the region of the vesicle occupied by the components with positive spontaneous curvature  $c_0^A$ , and  $c_0^B = 0.0$ , respectively. The lines meet at the inflection point of the hyperbolic tangent  $s_0$ . The profiles are presented for the total concentration  $\phi_{\text{tot}} = 0.25$  and for the spontaneous curvature (a)  $c_0^A = 1.00$ , (b)  $c_0^A = 2.00$ , and (c)  $c_0^A = 2.56$ .



**Figure 8.** The spontaneous curvature profiles  $c_0(s)$  (solid lines) and the local curvature  $c_1(s) + c_2(s)$  (dashed lines) for prolate vesicles with the reduced volume v = 0.655. s is the arclength. The profiles presented here start at the pole of the vesicles s = 0 and end at the equator of the vesicles  $s = L_s/2$ . The profiles are presented for the total concentration  $\phi_{\text{tot}} = 0.25$  and for the spontaneous curvature (a)  $c_0^A = 1.00$ , (b)  $c_0^A = 2.00$ , and (c)  $c_0^A = 2.56$ .

smooth function of  $c_0^{\rm A}$ . The local curvature and the spontaneous curvature do not overlap. Therefore, the energy cannot be very small for the prolate vesicles with domains.

All the calculations presented here are performed for the reduced volume v = 0.655. When the reduced volume is increased, a vesicle becomes more spherical, and the distribution of the local curvatures becomes more uniform. Thus, for the reduced volume close to 1, the separation of components due to the difference of the spontaneous curvatures should be difficult. One may expect that the interface will be large. However, decreasing the reduced volume should cause better separation and sharpening of the interface, since it would be possible to deform the shape of the vesicle to create regions with significantly different spontaneous curvatures. Thus, by deflating or inflating the vesicle, it may be possible to induce separation or mixing of the components which have different spontaneous curvatures. If the spontaneous curvature and the reduced volume are kept constant and the size of the vesicle is increased by increasing its surface area, the shape of the vesicle

and the distribution of components will change in a nontrivial way. If the unit length is set to the inverse of the spontaneous curvature instead of the radius of the sphere of the same surface area as the vesicle, then the results presented here will also describe the situation for variable size of the vesicle at conditions of constant spontaneous curvature and reduced volume. All the lengths would have to be rescaled by the spontaneous curvature.

# 4. Summary and Conclusions

We consider the model situation of a membrane with coherent domains formed by membrane components. The properties of components are characterized by the spontaneous curvatures. The domains are separated by the interface of nonzero width. The distribution of the components is an extra degree of freedom which can be exploited to minimize the bending energy. The change of the spontaneous curvature of one component (for example, due to a change of temperature) may lead to mixing or demixing. On the other hand, the change of the vesicle shape may be exploited to change the distribution of the components; for example, it may be used to induce the segregation of components. It has been shown that the interface width is narrow when the difference between the spontaneous curvature is small, and it grows instantly when the difference becomes large enough. The bending energy is lowered by widening the interface when the difference of the spontaneous curvatures of components is large. The change of the interface width between the domains may indicate the tendency of the membrane components to mixing and demixing.

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