



## Peng-Robinson Cubic Equation of State Based on Key Group Contribution and Calculation of Nitrogen Gas Solubility in MMA Dimer

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### ABSTRACT

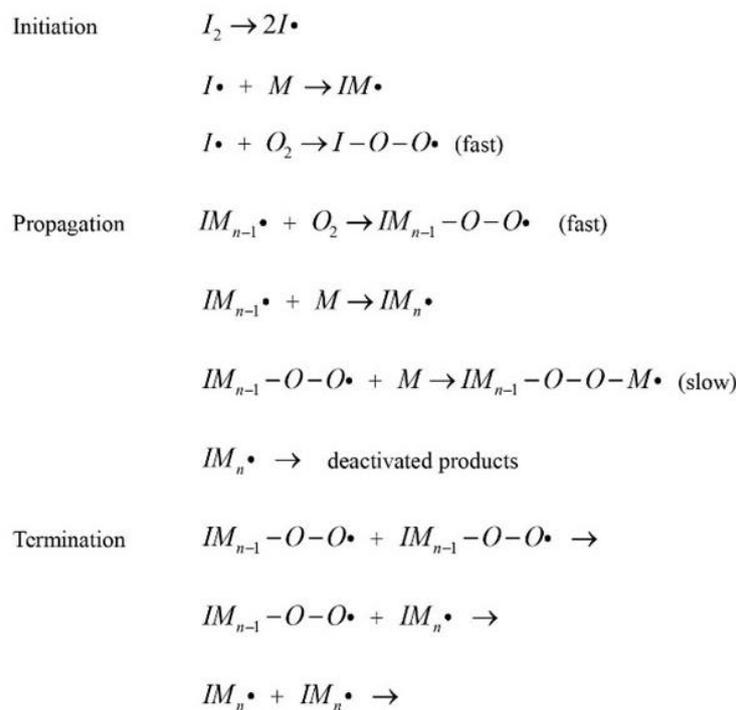
Previously authors have reported facts that nitrogen ( $N_2$ ) and oxygen solubilities in styrene is the same as those in benzene and divinylbenzene at 303 K. Though the three compounds have an atomic composition,  $(CH)_n$  ( $n=6, 8$  and  $10$ ), the gas solubilities are thought to depend on the number of aromatic carbons in the solution. Then, authors named it 'a key group in solubility'. In this research, the key group was investigated for  $N_2$  solubility in methyl methacrylate (MMA) and its dimer, ethylene glycol dimethacrylate (EGDMA). Therefore, the calculations were carried out by Peng-Robinson (PR) equation of state based on group contribution methods. The experimental data employed were those of Lai *et al.*, where  $N_2$  solubility are reported in MMA at 303 K. The  $N_2$  solubility in EGDMA was assumed to be double of that in MMA at 303 K, because EGDMA has two MMA units in the molecule. Two types of group contribution methods were proposed to calculate  $N_2$  solubility in EGDMA. One was for the critical temperature and pressure proposed by Joback and Reid. Using these properties, the attractive and excluded volume parameters in PR equation were evaluated for EGDMA. Other was similar to a method proposed by Orbey and Sandler. The excluded volume parameter in PR equation can be evaluated from those of MMA by multiplying the number of repeating units, and the attractive by multiplying the squared number. Instead of the method, the powers were proposed to be  $3/4$  and  $3/2$  for the excluded volume and attractive parameters, respectively. The powers were come from a scaling theory by de Gennes. The binary parameter for  $N_2$  – EGDMA was also set to  $k_{12} = 0.224$ , which was the same as that for  $N_2$  – MMA. The calculated  $N_2$  solubility in EGDMA was far smaller than the hypothetical  $N_2$  solubility in EGDMA at 303 K. Otherwise, to reproduce the hypothetical  $N_2$  solubility, a quite different value,  $k_{12} = -0.044$ , was necessary for the method by Joback and Reid. The results suggested that a key group for gas solubility will not be accepted in MMA.

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## 1. Introduction

Free radical polymerization is a common method for synthesizing polymers from vinyl monomers. Figure 1 shows the reaction scheme of free radical polymerization. It is composed of some elemental reactions [1,2], and divided into three steps, that is, initiation, propagation, and termination. If oxygen ( $O_2$ ) is dissolved in the solution, propagation will be affected with the  $n$ -mer free radical,  $IM_n \cdot$  [3-6] that will be converted to peroxide radical,  $IM_n-O-O \cdot$ , such that the reaction rate will be far larger than that in the absence of oxygen for which formation of the peroxide radical is slow. Therefore, usual propagation will not occur until oxygen dissolved in the solution is depleted and converted to peroxide radical. Thus, presence of oxygen molecules is well known to act as an inhibitor in radical polymerizations. To avoid oxygen inhibition, the monomer solution is saturated with nitrogen ( $N_2$ ) or argon (Ar), which is a procedure often used in polymerizations carried out in the laboratory.



**Fig. 1.** Reaction scheme of radical polymerization of vinyl monomer and formation of peroxide by oxygen dissolved in solution;  $I_2$  : initiator;  $M$ : vinyl monomer

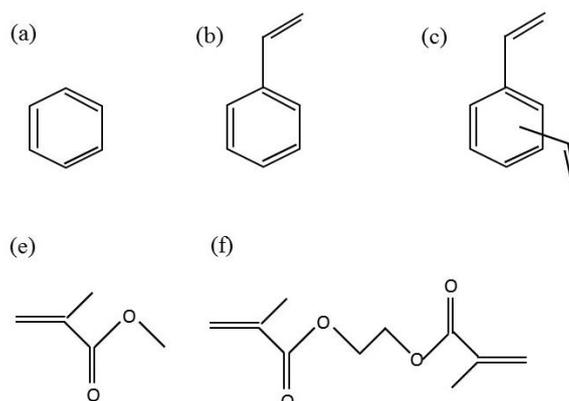
Styrene and methyl methacrylate (MMA) are the most popular vinyl monomers, and the bulk and the solution polymerization are widely employed in industry. For the design of the polymerization process, gas solubility data are necessary. In the previous research, the authors have reported  $N_2$  and  $O_2$  solubility in benzene, styrene and divinyl benzene at (293-303) K [7].

Figure 2 shows the molecular structure of benzene, styrene, and divinylbenzene. Benzene, styrene, and divinylbenzene correspond to the solvent, the monomer, and the cross linker with the same compositional formula  $(CH)_n$  ( $n=6, 8, 10$ ). If the solubility depends on the number of (CH) groups in the solution, the gas solubility would be evaluated in the various solutions containing not only benzene, styrene, and divinylbenzene but polystyrene.

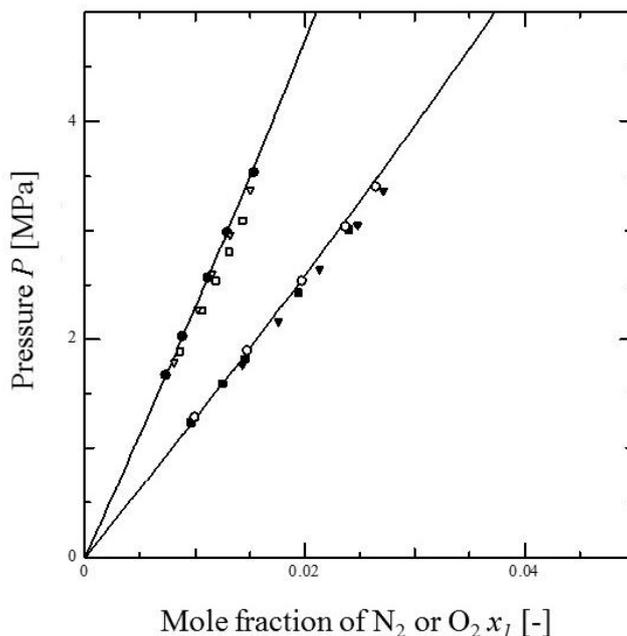
Figure 3 provides a comparison of nitrogen and oxygen solubilities in benzene, styrene and divinylbenzene at 313 K. Linear dependence in pressure was also observed for N<sub>2</sub> and O<sub>2</sub> solubilities in the three compounds, and it followed Henry's law at least up to 4 MPa. Surprisingly, the N<sub>2</sub> solubility in benzene was almost the same as that in styrene and divinylbenzene with similar trends also being observed for oxygen. Before the measurements, it was expected that the gas solubility in (CH) unit might be the same and that the correlation, using a group contribution method, could be available. However, the experimental data were found to depend mainly on the number of aromatic rings in the molecule. Therefore, the authors named the aromatic ring as a 'key group structure' in gas solubility. Successively, N<sub>2</sub> solubilities in MMA have been also reported at (293-313) K in the previous research [8]. Then, a linear dependence in pressure that followed Henry's law was also observed for N<sub>2</sub> and O<sub>2</sub> solubilities in MMA. Therefore, in this research, the authors investigated whether a key group structure is existing in MMA by using a cubic equation of state, Peng-Robinson (PR) [9]. Ethylene glycol dimethylacrylate (EGDMA) was selected as a dimer of MMA. The molecular structures of MMA and EGDMA are shown in Figure 2. EGDMA is composed of two MMA units. If a key group structure is in MMA molecule, gas solubility in EGDMA were expected to be twice that in MMA.

Gas solubility, vapor-liquid equilibria (VLE) and the related applications have been intensively reported for carbon dioxide (CO<sub>2</sub>) to apply to new technologies [10-15]. However, there are not so many researches of solubility and VLE for CO<sub>2</sub> in MMA or EGDMA. Lora and McHugh [16] and Uzun *et al.*, [17] have reported VLE for CO<sub>2</sub>-MMA, and Zwolak *et al.*, [18] have also reported CO<sub>2</sub> solubility in MMA. Kim *et al.*, [19] and Cho *et al.*, [20] reported CO<sub>2</sub> solubility in EGDMA. However, the available data, for N<sub>2</sub> and O<sub>2</sub> solubility in MMA, are just our previous research [8]. For N<sub>2</sub> and O<sub>2</sub> solubility in EGDMA, there is no available data in the literature.

In this research, two group contribution methods were proposed for EGDMA to estimate the parameters in PR equation. The calculations, using the methods, were compared with hypothetical N<sub>2</sub> solubility data in EGDMA at 313.18 K.



**Fig. 2.** Chemical structure of (a) benzene, C<sub>6</sub>H<sub>6</sub>, (b) styrene, C<sub>8</sub>H<sub>8</sub>, (c) Divinylbenzene, C<sub>10</sub>H<sub>10</sub>, (d) MMA, C<sub>5</sub>H<sub>8</sub>O<sub>2</sub> and (e) EGDMA, (C<sub>5</sub>H<sub>7</sub>O<sub>2</sub>)<sub>2</sub>



**Fig. 3.** Comparison of N<sub>2</sub> and O<sub>2</sub> solubilities in benzene, styrene, and divinylbenzene around 313 K [7]; (□): N<sub>2</sub> in benzene at 313.24 K; (●): N<sub>2</sub> in styrene at 313.30 K; (△): N<sub>2</sub> in divinylbenzene at 313.22 K; (■): O<sub>2</sub> in benzene at 313.23 K; (○): O<sub>2</sub> in styrene at 313.19 K; (▲): O<sub>2</sub> in divinylbenzene 313.24 K

## 2. Methodology

### 2.1 PR Equation of State

PR equation of state [9] have been widely used in process simulators not only for industry but also for research and education, and it is given by

$$P = \frac{RT}{v-b} - \frac{a}{v^2 + 2bv - b^2} \quad (1)$$

where  $a$  and  $b$  are attractive and excluded volume parameters of a pure compound. These are evaluated by applying corresponding state theory as follows

$$a = 0.45724 \frac{R^2 T_c^2}{P_c} \left[ 1 + \kappa \left\{ 1 - \left( \frac{T}{T_c} \right)^{1/2} \right\} \right]^2 \quad (2)$$

$$b = 0.07780 \frac{RT_c}{P_c} \quad (3)$$

$$\kappa = 0.37464 + 1.54226\omega - 0.26992\omega^2 \quad (4)$$

where  $T_c$  and  $P_c$  are the critical temperature and pressure of pure compound.  $\omega$  is acentric factor, which is obtained from temperature dependence of saturated vapor pressure [21]

$$\omega = -\log_{10} P^s \Big|_{T/T_c=0.7} - 1.000 \quad (5)$$

Stryjek and Vera have proposed a modified version of PR (PRSV) equation, and improved the reliability for saturated vapor pressure [22]. Though PRSV equation has the same function form as that of PR equation, the estimation of  $a$  and  $b$  is slightly different from that of PR equation

$$a = 0.457235 \frac{R^2 T_c^2}{P_c} \left[ 1 + \kappa \left\{ 1 - \left( \frac{T}{T_c} \right)^{1/2} \right\} \right]^2 \quad (6)$$

$$b = 0.077796 \frac{RT_c}{P_c} \quad (7)$$

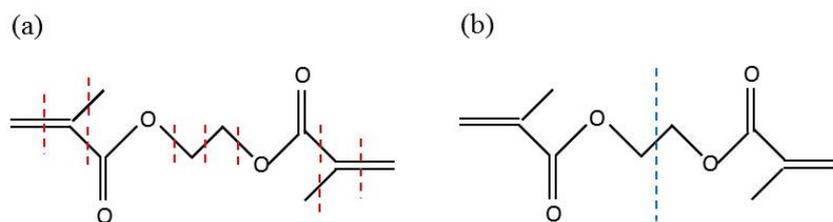
$$\kappa = \kappa_0 + \kappa_1 \left[ 1 + \left( \frac{T}{T_c} \right)^{1/2} \right] \left[ 0.7 - \frac{T}{T_c} \right] \quad (8)$$

$$\kappa_0 = 0.378893 + 1.4897153\omega - 0.171318\omega^2 + 0.0196554\omega^3 \quad (9)$$

where  $\kappa_1$  is a parameter, which is available in the literature [22]. Concerning gas solubility in this research, the parameter,  $\kappa_1$ , is provided just for N<sub>2</sub>, O<sub>2</sub>, and benzene. So, the parameters,  $a$  and  $b$ , are estimated from the three properties,  $T_c$ ,  $P_c$  and  $\omega$  as shown in Eqs.(2)-(4). However, there is no available data of  $T_c$ ,  $P_c$  and  $\omega$  for EGDMA.

## 2.2 Group Contribution Method

To estimate the two parameters,  $a$  and  $b$ , in PR equation for EGDMA, two group contribution methods were employed in this research. One was for the three properties,  $T_c$ ,  $P_c$  and  $\omega$ . The other was a direct estimation of  $a$  and  $b$  from those of the repeating unit, MMA. Figure 4 shows the groups in EGDMA based on the two group contribution methods.  $T_c$ ,  $P_c$  and  $\omega$  were evaluated by a group contribution method proposed by Joback and Reid [23].



**Fig.4.** Group in EGDMA; (a) For  $T_c$  and  $P_c$  (Joback and Reid [23]);  
 (b) for  $a$  and  $b$  (Orbay and Sandler [26])

According to the group contribution method, a molecule is divided into some functional groups, and  $T_c$  and  $P_c$  can be estimated as follows

$$T_c = \frac{T_b}{0.584 + 0.965 \sum \Delta_T - (\sum \Delta_T)^2} \quad (10)$$

$$P_c = \frac{1}{(0.113 + 0.0032 N_A - \sum \Delta_P)^2} \quad (11)$$

where  $\Delta_T$  and  $\Delta_P$  are group parameters for critical temperature and pressure, respectively, and they are available in the literature [23].  $T_b$  is normal boiling point, and  $N_A$  is the number of atoms in a molecule. For saturated vapor pressure, the following function was assumed from normal boiling point to critical point.

$$\log_{10} P^s = A + \frac{B}{T} \quad (12)$$

where  $A$  and  $B$  are constants. Applying Eq. (5), acentric factor,  $\omega$ , is obtained as follows [21,24,25]

$$\omega = \frac{1-0.7}{0.7} \times \frac{T_b/T_c}{1-(T_b/T_c)} \log_{10} \frac{P_c}{P_{atm}} - 1 \quad (13)$$

where  $T_b/T_c$  was evaluated by Eq. (10), and  $P_{atm}$  is a standard atmospheric pressure, 101.325 kPa. Orbey and Sandler [26] have also proposed an estimation of  $a$  and  $b$  for polymer by using those for repeating unit, monomer. The  $a$  and  $b$  are given by

$$a_{polymer} = \left( \frac{M_{w,polymer}}{M_{w,monomer}} \right)^2 a_{monomer} \quad (14)$$

$$b_{polymer} = \left( \frac{M_{w,polymer}}{M_{w,monomer}} \right) b_{monomer} \quad (15)$$

where  $M_{w,polymer}$  and  $M_{w,monomer}$  are molecular weights of polymer and monomer, respectively. The method can be applied to EGDMA, and it is thought to be an another group contribution method. However, considering the physical meaning of the excluded volume parameter,  $b$ , an improvement seems to be necessary. Then, the details are described later.

### 2.3 Mixing Rule

For the estimation of  $N_2$  solubility, PR / PRSV equation will be extended to the binaries by using mixing rule for  $a$  and  $b$ . Considering  $N_2$  and  $O_2$  solubilities shown in Figure 3, Henry's law is acceptable for the gas solubilities. Therefore, complex function forms will not be necessary in the mixing rule. So, conventional mixing rules, with simple function forms, were employed

$$a = \sum_{i=1}^2 \sum_{j=1}^2 x_i x_j (1 - k_{ij}) (a_i a_j)^{1/2} \quad (16)$$

$$b = \sum_{i=1}^2 x_i b_i \quad (17)$$

where  $k_{ij}$  ( $=k_{ji}$ ) is a binary interaction parameter. It is difficult to predict the values of  $k_{ij}$ . So, the values of  $k_{ij}$  for  $N_2$  solubility in EGDMA were determined by the two methods. One was the same value as that in MMA. The other was newly determined by fitting with the hypothetical  $N_2$  solubility data in EGDMA. The methods were described later.

### 3. Results and Discussion

#### 3.1 $N_2$ solubility in MMA and EGDMA

Figure 5 shows  $N_2$  solubility in MMA at 313.18 K, reported by Lai *et al.*, [8]. The data were obtained by a synthetic type apparatus, and  $O_2$  and Ar solubilities were also reported. Linear dependence in pressure that followed Henry's law was observed, and the similar tendency was also reported for  $O_2$  and Ar solubilities in MMA. Otherwise,  $N_2$  solubility has not been reported yet in EGDMA. Then,  $N_2$  solubility in EGDMA were assumed to be twice that in MMA. The hypothetical  $N_2$  solubility in EGDMA was also shown in Figure 5.

#### 3.2 Correlation for $N_2$ Solubility in MMA

PR / PRSV equation showed good reproducibility not only for  $N_2$  and  $O_2$  solubility in styrene but also for  $N_2$  solubility in MMA [7,8]. Table 1 lists the parameters for  $N_2$  and MMA for PR / PRSV equation. As listed in Table 1, the critical properties of  $N_2$  and MMA were from Stryjek and Vera [16] and Lora and McHugh [10], respectively.

The binary interaction parameter,  $k_{12}$ , was fitted with the experimental data to minimize the following objective function,  $O. F.$

$$O.F. = \sum_i (x_{1,cal} - x_{1,exp}) \quad (18)$$

Table 2 lists the binary interaction parameters.

**Table 1**

Critical properties for MMA and EGDMA

|          | Molecular weight<br>$M_w$ /- | Critical temperature<br>$T_c$ /K | Critical Pressure<br>$P_c$ /K | Acentric factor<br>$\omega$ /- | Parameter in PRSV eq.<br>$\kappa_1$ /- |
|----------|------------------------------|----------------------------------|-------------------------------|--------------------------------|--|
| Nitrogen | 28.013                       | <sup>a</sup> 126.200             | <sup>a</sup> 3.400            | <sup>a</sup> 0.03726           | <sup>a</sup> 0.01996                   |
| MMA      | 100.117                      | <sup>b</sup> 563.95              | <sup>b</sup> 3.68             | <sup>b</sup> 0.317             |  |
| EGDMA    | 198.22                       | <sup>c</sup> 692.0               | <sup>c</sup> 2.32             | <sup>c</sup> 0.679             |  |

<sup>a</sup>Ref. [22]; <sup>b</sup>Ref. [16]; <sup>c</sup>Group contribution method by Joback and Reid [23]

**Table 2**

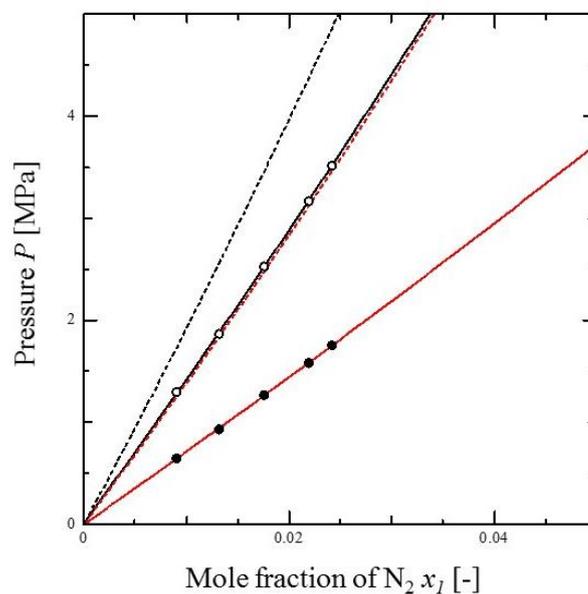
Binary interaction parameters in PR / PRSV equation

|                       | Binary interaction parameter $k_{12}$ ( $=k_{21}$ ) /- |
|-----------------------|--|
| $N_2$ (1) - MMA (2)   | 0.224  |
| $N_2$ (1) - EGDMA (2) | <sup>a</sup> -0.044                                    |

<sup>a</sup>for PR / PRSV equation using group contribution method by Joback and Reid [23] for EGDMA

### 3.3 Prediction for N<sub>2</sub> Solubility in EGDMA

Table 3 lists the parameters in the group contribution method for  $T_c$  and  $P_c$ , and Table 1 also lists the evaluated  $T_c$  and  $P_c$ . Then,  $N_A$  in Eq. (10), was set to be 28, and the normal boiling point,  $T_b$ , employed was that by Kim *et al.*, [19]. Consequently the value of  $T_c$  and  $P_c$  was ensured the same as those of Kim *et al.*, [19]. Figure 5 shows the prediction for N<sub>2</sub> solubility in EGDMA under the assumption of the same value of the binary interaction parameter as that for N<sub>2</sub> – EGDMA. As shown in Figure 5, the prediction for N<sub>2</sub> solubility in EGDMA was almost the same as that in MMA. Therefore, the predicted solubility was a half of the hypothetical N<sub>2</sub> solubility in EGDMA. Figure 5 also shows the result using the binary interaction parameter fitted with the hypothetical N<sub>2</sub> solubility in EGDMA. The value was listed in Table 2. The sign of the parameter was changed to be negative, so it means that the microscopic solution structure would be changed. Considering the similar structure in MMA and EGDMA, the phenomena will not to be accepted.



**Fig. 5.** Comparison of N<sub>2</sub> solubilities in MMA and EGDMA; (o) MMA at 313.18 K; (●) EGDMA at 313.18 K (hypothetical); (—): PR / PRSV equation for MMA; (---): PR /PRSV equation by Orbey and Sandler method with SAW model for EGDMA ( $k_{12}=0.224$ ); (---): PR /PRSV eq. by Joback and Reid method for EGDMA ( $k_{12}=0.224$ ); (—): PR / PRSV equation by Joback and Reid method for EGDMA ( $k_{12}=-0.044$ )

**Table 3**

Parameters for EGDMA in group contribution method by Joback and Reid [23]

| Group              | Number of group | Value of group parameter |            |
|--------------------|-----------------|--------------------------|------------|
|                    |                 | $\Delta_T$               | $\Delta_P$ |
| -CH <sub>3</sub>   | 2               | 0.0141                   | -0.0012    |
| -CH <sub>2</sub> - | 2               | 0.0189                   | 0.0000     |
| =CH <sub>2</sub>   | 2               | 0.0013                   | -0.0028    |
| =C<                | 2               | 0.0117                   | 0.0011     |
| -COO-              | 2               | 0.0481                   | 0.0005     |

Prior to the calculation by group contribution method by Orbey and Sandler [26], Eq. (14) and (15) were considered again from a view point of physical meaning by using a scaling model of de Gennes [21]. The parameter,  $b$ , is an excluded volume parameter. If that of  $n$ -mer is proportional to the degree of polymerization, it is converted to the rigid rod (RR) model as follows

$$L = nl \tag{19}$$

where  $L$  and  $l$  correspond to end-to-end distance, and length of repeating unit. Considering the flexibility of molecule of repeating unit, the evaluation,  $b = (M_{w,EGDMA} / M_{w,MMA})b_{MMA}$  seems to be an overestimation. Otherwise, in random walk (RW) model, end-to-end distance,  $L$ , is mathematically given by

$$L = n^{1/2}l \tag{20}$$

Therefore,  $b = (M_{w,EGDMA} / M_{w,MMA})^{1/2}b_{MMA}$  can be derived. However, it seems to be an underestimation because the over lapping is not allowed in the configuration. Then, self-avoiding walk (SAW) model was employed in this research.

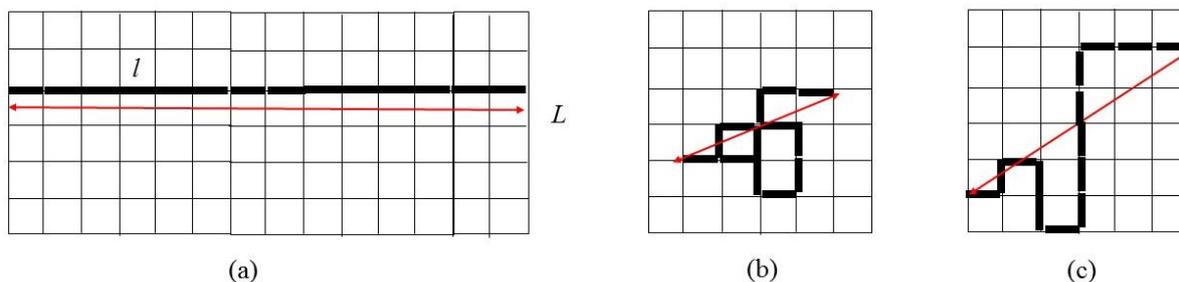
Figure 6 shows illustration of the three models [27]. In SAW model, the power for the number of repeating units will be smaller than that RR model, and larger than that of RW model. Consequently, the following relation was assumed as follows

$$a_{EGDMA} = \left( \frac{M_{w,EGDMA}}{M_{w,MMA}} \right)^{3/2} a_{MMA} \tag{21}$$

$$b_{EGDMA} = \left( \frac{M_{w,EGDMA}}{M_{w,MMA}} \right)^{3/4} b_{MMA} \tag{22}$$

where  $M_{w,EGDMA}$  and  $M_{w,MMA}$  are molecular weights of EGDMA and MMA, respectively.

Figure 5 shows the prediction for  $N_2$  solubility in EGDMA under the assumption of the same value of the binary interaction parameter as that for  $N_2 - EGDMA$ . As shown in Figure 5,  $N_2$  solubility predicted was far smaller than the hypothetical data. If the interaction parameter was fitted with the hypothetical data, the values will be smaller than  $k_{12} = -0.044$ . So, any prediction was not carried out in this research.



**Fig. 6.** Models of end to end distance in a molecule composed of some repeating units; (a) Rigid rod (RR); (b) Random walk (RD); (c) Self-avoiding walk (SAW)

## 4. Conclusions

Two group contribution models were proposed for N<sub>2</sub> solubility prediction in EGDMA, dimer of MMA. The model by Joback and Reid [17] showed the same N<sub>2</sub> solubility as that in MMA by using a common binary interaction parameter,  $k_{12}=0.224$ . Considering the calculation results, a key group for gas solubility will not be accepted in MMA. The result was different from that in styrene. However, the data of EGDMA is hypothetical ones, so the actual experimental data of N<sub>2</sub> solubility is required in EGDMA for further investigation of key group in gas solubility.

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