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On the lower and upper bounds for general Randić index of chemical (n, m)-graphs

Xueliang Li1,2, Xueqin Wang1*and Bing Wei1

¹Department of Mathematics The University of Mississippi Oxford, MS 38677, USA and ²Center for Combinatorics Nankai University Tianji 300071, China

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Abstract

A chemical (n, m)-graph is a connected graph of order n, size m and maximum degree at most 4. The general Randić index of a graph is defined as the sum of the weights $[d(u)d(v)]^{\alpha}$ of all edges uv of the graph, where α is any real number and d(u) is the degree of a vertex u. In this paper, we give the lower and upper bounds for general Randić index of chemical (n, m)-graphs.

A graph of order n and size m is called an (n, m)-graph. A connected graph is called chemical if its maximum degree is at most 4.

The Randić index of a graph G is defined in [6] as

$$\chi(G) = \sum_{uv} \frac{1}{[d(u)d(v)]^{1/2}},$$
(1)

^{*}Corresponding author: xueqin@olemiss.edu

where uv runs over all edges of G, and d(u) is the degree of a vertex u.

The general Randić index is defined in [1, 2] as follows

$$\chi_{\alpha}(G) = \sum_{uv \in E(G)} [d(u)d(v)]^{\alpha}, \qquad (2)$$

where α is a real number. The authors of [3, 4] studied the lower and upper bounds for Randić index (i.e. $\alpha = -1/2$) of chemical (n, m)-graphs, while the authors of [5] gave the bounds for chemical trees with $\alpha = -1$. The focus of this paper is on the lower and upper bounds for general Randić index (i.e. any real number α) of chemical (n, m)-graphs.

Suppose that G is a chemical (n, m)-graph. Let x_{ij} denote the number of edges each having end-vertices of degrees i and j respectively, for $1 \le i \le j \le 4$. Note that G is connected, x_{11} is thus zero for n > 2. Therefore, (2) can be presented as

$$\chi_{\alpha}(G) = \sum_{1 \le i \le j \le 4} (ij)^{\alpha} x_{ij}$$

$$= 2^{\alpha} x_{12} + 3^{\alpha} x_{15} + 4^{\alpha} (x_{14} + x_{22}) + 6^{\alpha} x_{23} + 8^{\alpha} x_{24}$$

$$+ 9^{\alpha} x_{33} + 12^{\alpha} x_{34} + 16^{\alpha} x_{44}.$$

If we count the number of vertices and the number of edges in two different ways, respectively, we would then have the following identities,

$$\sum_{1 \le i \le j \le 4} \left(\frac{1}{i} + \frac{1}{j} \right) x_{ij} = n \tag{3}$$

$$\sum_{1 \le i \le j \le 4} x_{ij} = m \tag{4}$$

First, we choose two different variables x_{ab} and x_{cd} among the x_{ij} 's except x_{11} , and then solve them from the above linear equations,

$$x_{ab} = \gamma \left[n - \left(\frac{1}{c} + \frac{1}{d} \right) m + \sum_{ab \neq ij \neq cd} \left(\frac{1}{c} + \frac{1}{d} - \frac{1}{i} - \frac{1}{j} \right) x_{ij} \right], \tag{5}$$

$$x_{cd} = -\gamma \left[n - \left(\frac{1}{a} + \frac{1}{b}\right)m + \sum_{ab \neq ij \neq cd} \left(\frac{1}{a} + \frac{1}{b} - \frac{1}{i} - \frac{1}{j}\right)x_{ij}\right],\tag{6}$$

where $\gamma = 1/(\frac{1}{a} + \frac{1}{b} - \frac{1}{c} - \frac{1}{d})$. Therefore, the general Randić index $\chi_{\alpha}(G)$ can be rewritten in form of x_{ij} 's except x_{ab} and x_{cd} ,

$$\begin{split} \chi_{\alpha}(G) &= \sum_{ab \neq ij \neq cd} (ij)^{\alpha} x_{ij} + (ab)^{\alpha} x_{ab} + (cd)^{\alpha} x_{cd} \\ &= \sum_{ab \neq ij \neq cd} (ij)^{\alpha} x_{ij} + \gamma (ab)^{\alpha} [n - (\frac{1}{c} + \frac{1}{d})m + \sum_{ab \neq ij \neq cd} (\frac{1}{c} + \frac{1}{d} - \frac{1}{i} - \frac{1}{j}) x_{ij}] \\ &- \gamma (cd)^{\alpha} [n - (\frac{1}{a} + \frac{1}{b})m + \sum_{ab \neq ij \neq cd} (\frac{1}{a} + \frac{1}{b} - \frac{1}{i} - \frac{1}{j}) x_{ij}] \\ &= \gamma n [(ab)^{\alpha} - (cd)^{\alpha}] + \gamma m [(cd)^{\alpha} (\frac{1}{a} + \frac{1}{b}) - (ab)^{\alpha} (\frac{1}{c} + \frac{1}{d})] \\ &+ \sum_{ab \neq ij \neq cd} [(ij)^{\alpha} + \gamma (\frac{1}{c} + \frac{1}{d} - \frac{1}{i} - \frac{1}{j}) (ab)^{\alpha} + \gamma (\frac{1}{i} + \frac{1}{j} - \frac{1}{a} - \frac{1}{b}) (cd)^{\alpha}] x_{ij} \\ &= \gamma n [(ab)^{\alpha} - (cd)^{\alpha}] + \gamma m [(cd)^{\alpha} (\frac{1}{a} + \frac{1}{b}) - (ab)^{\alpha} (\frac{1}{c} + \frac{1}{d})] \\ &+ \gamma \sum_{1 \leq i \leq j \leq 4} [\frac{1}{\gamma} (ij)^{\alpha} + (\frac{1}{c} + \frac{1}{d} - \frac{1}{i} - \frac{1}{j}) (ab)^{\alpha} + (\frac{1}{i} + \frac{1}{j} - \frac{1}{a} - \frac{1}{b}) (cd)^{\alpha}] x_{ij}. \end{split}$$

Let

$$B(ab, cd) = \frac{n[(ab)^{\alpha} - (cd)^{\alpha}] + m[(cd)^{\alpha}(\frac{1}{a} + \frac{1}{b}) - (ab)^{\alpha}(\frac{1}{c} + \frac{1}{d})]}{\frac{1}{a} + \frac{1}{b} - \frac{1}{c} - \frac{1}{d}}$$
(7)

and

$$R_{ij}(ab,cd) = \frac{1}{\gamma}(ij)^{\alpha} + (\frac{1}{c} + \frac{1}{d} - \frac{1}{i} - \frac{1}{j})(ab)^{\alpha} + (\frac{1}{i} + \frac{1}{j} - \frac{1}{a} - \frac{1}{b})(cd)^{\alpha}. \tag{8}$$

Then $\chi_{\alpha}(G)$ can be expressed as follows,

$$\chi_{\alpha}(G) = B(ab, cd) + \gamma \sum_{1 \le i \le j \le 4} R_{ij}(ab, cd) x_{ij}. \tag{9}$$

Our next aim is to determine whether there are some ab's and cd's such that $R_{ij}(ab,cd)$ are all non-negative or non-positive. Without loss of generality, we assume that $\gamma > 0$. If the answer is yes, for example, there is $(\overline{ab}, \overline{cd})$ such that $R_{ij}(\overline{ab}, \overline{cd})$ are non-positive. Then $B(\overline{ab}, \overline{cd})$ is an upper bound of the Randić index $\chi(G)$.

The forms of $R_{ij}(ab, cd)$ lead us to study the functions

$$S(ij,kl) = \frac{(ij)^{\alpha} - (kl)^{\alpha}}{(\frac{1}{i} + \frac{1}{2}) - (\frac{1}{k} + \frac{1}{1})}.$$
 (10)

For convenience, let S(ij,ij) = 0. Note that if $\alpha \ge 0$, then $S(ij,kl) \le 0$, and if $\alpha < 0$, then $S(ij,kl) \ge 0$.

We construct a symmetric matrix of elements S(ij,kl) defined in (10) and denote by S. Since S is symmetric, we only consider the upper triangular part of S here. An interesting lemma to determine all $(\underline{ab},\underline{cd})$'s and $(\overline{ab},\overline{cd})$'s which guarantee all $R_{ij}(\underline{ab},\underline{cd})$ non-negative and $R_{ij}(\overline{ab},\overline{cd})$ non-positive, respectively, yields as follows.

Lemma 1. There exist $(\overline{ab}, \overline{cd})$'s and $(\underline{ab}, \underline{cd})$'s such that $S(\overline{ab}, \overline{cd})$ is simultaneously minimal in its row and maximal in its column in the upper triangular part of S, and $S(\underline{ab}, \underline{cd})$ is simultaneously maximal in its row and minimal in its column, i.e.

$$S(\overline{ab}, \overline{cd}) \le S(\overline{ab}, kl), \text{ for } 1/\overline{a} + 1/\overline{b} > 1/k + 1/l,$$
 (11)

$$S(\overline{ab}, \overline{cd}) \ge S(ij, \overline{cd}), \text{ for } 1/i + 1/j > 1/\overline{c} + 1/\overline{d};$$
 (12)

and

$$S(\underline{ab}, \underline{cd}) \ge S(\underline{ab}, kl), \text{ for } 1/\underline{a} + 1/\underline{b} > 1/k + 1/l, \tag{13}$$

$$S(\underline{ab},\underline{cd}) \le S(ij,\underline{cd}), \text{ for } 1/i + 1/j > 1/\underline{c} + 1/\underline{d}. \tag{14}$$

The proof of Lemma 1 will be based on Lemma 3. Let us first verify that $(\underline{ab}, \underline{cd})$ and $(\overline{ab}, \overline{cd})$ satisfy that all $R_{ij}(\underline{ab}, \underline{cd})$ non-negative and $R_{ij}(\overline{ab}, \overline{cd})$ non-positive. Indeed, $R_{ij}(ab, cd)$ can be expressed in the following two forms:

$$R_{ij}(ab,cd) = -\frac{1}{\gamma}(\frac{1}{a} + \frac{1}{b} - \frac{1}{i} - \frac{1}{j})(S(ab,ij) - S(ab,cd))$$
 (15)

$$= \frac{1}{\gamma} (\frac{1}{i} + \frac{1}{j} - \frac{1}{c} - \frac{1}{d}) (S(ij, cd) - S(ab, cd))$$
 (16)

If $1/\overline{a} + 1/\overline{b} > 1/i + 1/j$, by (11), (15), $R_{ij}(\overline{ab}, \overline{cd}) \le 0$; Otherwise $1/\overline{a} + 1/\overline{b} \le 1/i + /j$. Note that $1/\overline{c} + 1/\overline{d} < 1/\overline{a} + 1/\overline{b}$. Thus, $1/i + 1/j > 1/\overline{c} + 1/\overline{d}$, and by (12), (16), we have $R_{ij}(\overline{ab}, \overline{cd}) \le 0$, too. The argument in similar manner leads that $R_{ij}(\underline{ab}, \underline{cd}) \ge 0$.

Theorem 2. The general Randić index $\chi(G)$ has the following bounds:

$$B(\underline{ab}, \underline{cd}) \le \chi(G) \le B(\overline{ab}, \overline{cd})$$
 (17)

for chemical (n,m)-graphs, where B(ab,cd) is defined in (7), $(\underline{ab},\underline{cd})$ and $(\overline{ab},\overline{cd})$ are defined in Lemma 1.

If $\alpha = -1$, then the matrix S is

1.00 0.50 0.50 0.50

```
0.33
                              1.00
                                    0.25
                                          0.33
                                                 0.36
                                                       0.33
                                    0.00 0.20
                                                 0.25
                                                       0.24
                                                             0.25
                                                                   0.25
                              0.00
                                    0.00 0.50
                                                 0.50
                                                                   0.38
                              0.20
                                    0.50 0.00
                                                 0.50
                                                       0.33
                                                                   0.31
                 0.50 0.36
                              0.25
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                                                       0.17
                                                             0.25
                                                                   0.25
                 0.47 0.33
                              0.24
                                                                   0.29
                                    0.42
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                                                             0.33
                              0.25
                                                 0.25
                                                       0.33
                                                                   0.25
                                    0.40
                                          0.33
                                                             0.00
                 0.44
                       0.33
                              0.25
                                    0.38
                                          0.31
                                                 0.25
                                                       0.29
                                                             0.25
                                                                   0.00
(\overline{ab}, \overline{cd}):
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                                          0.50
                                                 0.50
                                                       0.47
                                                             0.45
                                                                   0.44
                 0.00
                       1.00
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                 0.50 0.33
                                                                   0.31
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                                                             0.00
                        0.33
                              0.25
                                    0.38
                                          0.31
                                                 0.25
                                                       0.29
                                                             0.25
                                                                   0.00
(ab, cd):
                                                 0.50
                              1.00
                                    0.50
                                          0.50
                                                       0.47
                       0.00
                              1.00
                                    0.25
                                          0.33
                                                 0.36
                                                       0.33
                                                             0.33
                                                                   0.33
                      1.00
                              0.00
                                    0.00
                                          0.20
                                                 0.25
                                                       0.24
                  0.50 0.25
                                   0.00
                                          0.50
                                                 0.50
                                                                   0.38
                              0.00
                                                       0.42
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                             0.20
                                   0.50 0.00
                                                 0.50
                                                                   0.31
                             0.25
                                    0.50 0.50
                                                 0.00
                                                       0.17
                                                                   0.25
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                                    0.42 0.33
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                                    0.40 \ 0.33 \ 0.25
                                                       0.33
                                                            0.00
                             0.25
                                   0.38 0.31 0.25 0.29 0.25
                 0.44 0.33
```

Thus, $(\overline{ab}, \overline{cd}) = (12, 44)$, and we may choose $(\underline{ab}, \underline{cd}) = (14, 44)$. Then, the upper bound is B(12, 44) = (14n - 5m)/32 and the lower bound is B(34, 44) = (4n - m)/16, where the lower bound for chemical trees coincides with the result of [5].

As we observed in the examples, there are possibly more than one value for both $(\overline{ab}, \overline{cd})$ and $(\underline{ab}, \underline{cd})$, however, one of $(\overline{ab}, \overline{cd})$'s would fall in the first row and one of $(\underline{ab}, \underline{cd})$'s would fall in the last column. Based on this fact, we have a constructive proof for Lemma 1. To avoid the mess of notations, we are going to prove a statement which simplifies Lemma 1. We also present it as a lemma.

Illustrative examples are given to show the idea of choice of $(\underline{ab}, \underline{cd})$ and $(\overline{ab}, \overline{cd})$. As reported in [3, 4], a bound of the Randić index is as follows

$$\frac{4n+m}{12} \le \chi(G) \le \frac{(2\sqrt{2}-2)n - (3-2\sqrt{2})m}{2}.$$
 (18)

In this case, $\alpha = -1/2$, and $\{12, 13, 14, 22, 23, 24, 33, 34, 44\}$ are listed in the order based on the values (1/i + 1/j)'s. The matrix S is obtained as follows.

 $(\overline{ab}, \overline{cd})$:

$$\begin{pmatrix} 0.00 & 0.78 & 0.83 & \overline{0.41} & 0.45 & 0.47 & 0.45 & 0.46 & 0.46 \\ 0.78 & 0.00 & 0.93 & 0.23 & 0.34 & 0.38 & 0.37 & 0.38 & 0.39 \\ 0.83 & 0.93 & 0.00 & 0.00 & 0.22 & 0.29 & 0.29 & 0.32 & 0.33 \\ 0.41 & 0.23 & 0.00 & 0.00 & 0.55 & 0.59 & 0.50 & 0.51 & \overline{0.50} \\ 0.45 & 0.34 & 0.22 & 0.55 & 0.00 & 0.66 & 0.45 & 0.48 & 0.47 \\ 0.47 & 0.38 & 0.29 & 0.59 & 0.66 & 0.00 & 0.24 & 0.39 & 0.41 \\ 0.45 & 0.37 & 0.29 & 0.50 & 0.45 & 0.24 & 0.00 & 0.54 & \overline{0.50} \\ 0.46 & 0.38 & 0.32 & 0.51 & 0.48 & 0.39 & 0.54 & 0.00 & 0.46 \\ 0.46 & 0.39 & 0.33 & 0.50 & 0.47 & 0.41 & 0.50 & 0.46 & 0.00 \\ \end{pmatrix}$$

(ab, cd):

$$\begin{pmatrix} 0.00 & 0.78 & \overline{0.83} & 0.41 & 0.45 & 0.47 & 0.45 & 0.46 & 0.46 \\ 0.78 & 0.00 & 0.93 & 0.23 & 0.34 & 0.38 & 0.37 & 0.38 & 0.39 \\ 0.83 & 0.93 & 0.00 & 0.00 & 0.22 & 0.29 & 0.29 & 0.32 & \overline{0.33} \\ 0.41 & 0.23 & 0.00 & 0.00 & 0.55 & 0.59 & 0.50 & 0.51 & 0.50 \\ 0.45 & 0.34 & 0.22 & 0.55 & 0.00 & 0.66 & 0.45 & 0.48 & 0.47 \\ 0.47 & 0.38 & 0.29 & 0.59 & 0.66 & 0.00 & 0.24 & 0.39 & 0.41 \\ 0.45 & 0.37 & 0.29 & 0.50 & 0.45 & 0.24 & 0.00 & 0.54 & 0.50 \\ 0.46 & 0.38 & 0.32 & 0.51 & 0.48 & 0.39 & 0.54 & 0.00 & 0.46 \\ 0.46 & 0.39 & 0.33 & 0.50 & 0.47 & 0.41 & 0.50 & 0.46 & 0.00 \\ \end{pmatrix}$$

Thus, let $(\overline{ab}, \overline{cd}) = (12, 22)$. Similarly, let $(\underline{ab}, \underline{cd}) = (14, 44)$. Therefore, we obtain that the upper bound of $\chi(G)$, $B(12, 22) = [(2\sqrt{2} - 2)n + (3 - 2\sqrt{2})m]/2$ and the lower bound B(14, 44) = (4n + m)/12.

Lemma 3. Given an ordered sequence of numbers $a_1 > \cdots > a_n > 0$ and a sequence of numbers b_1, \cdots, b_n . A symmetric $n \times n$ matrix E is defined with entries

$$e_{ij} = \begin{cases} \frac{b_i - b_j}{a_i - a_j} & \text{if } i \neq j; \\ 0 & \text{if } i = j. \end{cases}$$

Then

- e_{1j0} = min_{j≠1} e_{1j} is simultaneously minimal in its row and maximal in its column in the upper triangular part of E; and
- e_{ion} = min_{i≠n} e_{in} is simultaneously maximal in its row and minimal in its column in the upper triangular part of E.

Proof. We only need to prove the first part. Indeed, we need to check that

$$e_{1j_0} \ge e_{ij_0}$$
 for $i < j_0$,

which is equivalent to

$$e_{1i} \ge e_{1i0}$$
 for $i < j_0$.

Since e_{1j_0} is minimal in its row, the above inequality holds.

Indeed, let a_1, \dots, a_9 in Lemma 3 be the order of the numbers (1/i+1/j)'s. We can find at least one $(\overline{ab}, \overline{cd})$ and one $(\underline{ab}, \underline{cd})$ which are defined in Lemma 1 for each real number α . Applying Lemma 3 and Theorem 2, the bounds for the general Randić index of chemical (n, m)-graphs yield. We summarize them as the following theorem. Let $\alpha_1, \alpha_2, \alpha_3$ be the non-zero roots of equations S(12, 22) = S(12, 44), S(12, 14) = S(12, 44), S(14, 44) = S(34, 44), respectively. We can use Maple to calculate the numerical values of them easily: $\alpha_1 = -.6942419136, \alpha_2 = .3815886463, \alpha_3 = -1.0$. See Figures 1, 2 and 3.

Theorem 4. The general Randić index $\chi(G)$ of chemical (n, m)-graphs has the following lower and upper bounds

1. $-\infty < \alpha \le \alpha_1 \& \alpha_2 < \alpha < \infty$

$$\chi(G) \le (2^{\alpha} - 16^{\alpha})n + (\frac{3}{2}16^{\alpha} - 2^{\alpha - 1})m;$$
 (19)

2. $\alpha_1 < \alpha \le 0$

$$\chi(G) \le (2^{\alpha+1} - 2 \cdot 4^{\alpha})n + (3 \cdot 4^{\alpha} - 2^{\alpha+1})m; \tag{20}$$

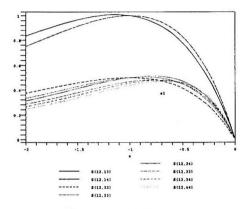


Figure 1: critical point α_1

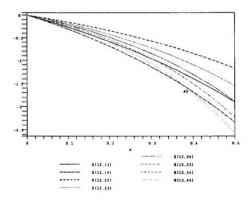


Figure 2: critical point α_2

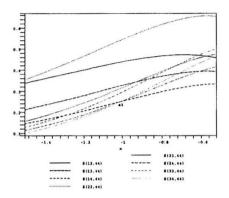


Figure 3: critical point α_3

3. $0 < \alpha \le \alpha_2$

$$\chi(G) \le (2^{\alpha+2} - 4^{\alpha+1})n + (6 \cdot 4^{\alpha} - 5 \cdot 2^{\alpha})m; \tag{21}$$

4. $-\infty < \alpha < \alpha_3 \& 0 \le \alpha < \infty$

$$\chi(G) \ge (12^{\alpha+1} - 12 \cdot 16^{\alpha})n + (7 \cdot 16^{\alpha} - 6 \cdot 12^{\alpha})m; \tag{22}$$

5. $\alpha_3 \leq \alpha < 0$

$$\chi(G) \ge \frac{(4^{\alpha+1} - 4 \cdot 16^{\alpha})n + (5 \cdot 16^{\alpha} - 2 \cdot 4^{\alpha})m}{3}.$$
(23)

Proof. We can verify that S(12,22), S(12,14), S(12,44) are smallest among S(12,kl)'s in each corresponding interval of α : $\alpha_1 < \alpha \leq 0$, $-\infty < \alpha \leq \alpha_1$ & $\alpha_2 < \alpha < \infty$, $0 < \alpha \leq \alpha_2$; and S(14,44), S(34,44) are smallest among S(ij,44)'s in each corresponding interval of α : $\alpha_3 \leq \alpha < 0$, $-\infty < \alpha < \alpha_3$ & $0 \leq \alpha < \infty$. By Lemma 3 and Theorem 2, we have the above results.

It is not difficult for us to give examples to show that some of the above bounds are best possible for some values of α . In most cases, we do not know yet whether or not the

above bounds are best possible. However, one can improve them by discussing them case by case similar to the idea in [3, 4].

To end this paper, we point out that we can employ the same method to give a lower and an upper bound for the general Randić index of general (n, m)-graphs with maximum degree at most k. For example, for $\alpha = -1$ the bounds are as follows

$$\frac{n}{k} - \frac{m}{k^2} \le \chi_{-1}(G) \le \frac{n(\frac{1}{2} - \frac{1}{k^2}) + m(\frac{3}{2k^2} - \frac{1}{k})}{\frac{3}{2} - \frac{2}{k}}.$$

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