Flow Polynomial of some Dendrimers

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ABSTRACT. Suppose $G$ is an $n$–vertex and $m$–edge simple graph with edge set $E(G)$. An integer–valued function $f: E(G) \rightarrow \mathbb{Z}$ is called a flow. Tutte was introduced the flow polynomial $F(G, \lambda)$ as a polynomial in an indeterminate $\lambda$ with integer coefficients by

$$F(G, \lambda) = (-1)^{|E(G)|} \sum_{S \subseteq E(G)} (-1)^{|S|} \lambda^{n-m+c(G:S)},$$

where $c(G:S)$ is the number of connected components of $G$ and $(G : S)$ denotes the spanning subgraph of $G$ with edge set $S$. In this paper the Flow polynomial of some dendrimers are computed.

Keywords: Flow polynomial, dendrimer, graph.

1 INTRODUCTION

A simple graph $G = (V, E)$ is a finite nonempty set $V(G)$ of objects called vertices together with a set $E(G)$ of unordered pairs of distinct vertices of $G$ called edges. In chemical graphs, the vertices correspond to the atoms and the edges represent the chemical bonds. If $x, y \in V(G)$ then the distance $d(x,y)$ between $x$ and $y$ is defined as the length of a minimum path connecting $x$ and $y$.

For a simple graph $G$, integer–valued function $f: E(G) \rightarrow \mathbb{Z}$ is called a flow. Tutte was introduced the flow polynomial $F(G, \lambda)$ as a graph function and as a polynomial in an indeterminate $\lambda$ with integer coefficients by

$$F(G, \lambda) = (-1)^{|E(G)|} \sum_{S \subseteq E(G)} (-1)^{|S|} \lambda^{n-m+c(G:S)},$$

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where $c(G:S)$ is the number of connected components of $G$ and $(G : S)$ denotes the spanning subgraph of $G$ with edge set $S$ [1, 5–8]. At $x = 0$, the Tutte polynomial specializes to the flow polynomial studied in combinatorics. He proved that

$$F(G, \lambda) = (-1)^{|E|+|V|+c(G)}T(G, 0, 1 - \lambda),$$

where $T(G, x, y)$ is the Tutte polynomial of graph $G$.

We denote the complete graph, the cycle and the path of order $n$ by $K_n$, $C_n$ and $P_n$, respectively.

## 2 The Flow Polynomial of Graphs

In this section we compute the flow polynomial of an infinite class of special type D of dendrimers. Dendrimers are complex macromolecules with very well–defined chemical structures. They consist of three major architectural components: core, branches and end groups. The topological study of these macromolecules is the subject of some recent papers [2–4]. For the sake of completeness, we mention here six results from [5] which are important in our calculations.

**Theorem A.** $F(G, \lambda)$ is a polynomial of degree $t = t(G)$. The coefficient of $\lambda^t$ is $(-1)^t$ and all terms in $F(G, \lambda)$ have the same sign.

**Theorem B.** If $G$ has no edges, then $F(G, \lambda) = 1$ and if $G$ has a bridge, then $F(G, \lambda) = 0$.

**Theorem C.** If $G$ consists of two graphs $H$ and $K$ which are either disjoint or have a single vertex in common, then $F(G, \lambda) = F(H, \lambda)F(K, \lambda)$.

**Theorem D.** If $G$ is a cycle, then $F(G, \lambda) = \lambda - 1$.

**Theorem E.** $F(G, \lambda)$ is a topological invariant and hence any two homeomorphic graphs will have the same flow polynomial.

**Theorem F.** If $e$ is any edge of $G$, then $F(G, \lambda) = F(G-e, \lambda) - F(G.e, \lambda)$, where $G.e$ contracting the edge $e$.

**Theorem 1.** Let $G$ be a graph with two induced cycles $C_m$ and $C_n$ containing a common path $P_{t}$ without bridge edge. Then the Flow polynomial of $G$ is obtained as follows:

$$F(G, \lambda) = \left(F(C_{m-t+1}, \lambda)F(C_{n-t+1}, \lambda) + F(C_{m+n-2t+2}, \lambda)\right).$$
**Proof.** The graph $H$ has two induced cycles, $C_m$ and $C_n$, such that they have a path $P_t$ in common, see Figure 1. Let $P_t$: $v_1e_1v_2e_2 \ldots v_{t-1}e_{t-1}v_t$ be a common path between $C_m$ and $C_n$. Then we have

$$F(H, \lambda) = F(H/e_1, \lambda) + F(H - e_1, \lambda).$$

Since $H - e_1$ is a unicycle graph, then $F(H - e_1, \lambda) = F(C_{m+n-2t+2}, \lambda)$. By continuing this process, we have

$$F(H, \lambda) = F(H/e_1/e_2, \lambda) + F(H/e_1 - e_2, \lambda) + F(H - e_1, \lambda)$$

$$= F(H/e_1/e_2/e_3, \lambda) + F(H/e_1/e_2 - e_3, \lambda) + F(H/e_1 - e_2, \lambda) + F(H - e_1, \lambda)$$

$$\vdots$$

$$= F(H/e_1/e_2/e_3/\ldots/e_{t-1}, \lambda) + F(H/e_1/e_2/e_3/\ldots/e_{t-2} - e_{t-1}, \lambda) + F(H/e_1/e_2/e_3/\ldots/e_{t-3} - e_{t-2}, \lambda) + F(H/e_1/e_2/e_3/\ldots/e_{t-4} - e_{t-3}, \lambda) + \ldots$$

$$+ F(H/e_1/e_2 - e_3, \lambda) + F(H/e_1 - e_2, \lambda) + F(H - e_1, \lambda)$$

$$= F(C_m, \lambda) T(C_n, \lambda) + F(C_{m+n-2t+2}, \lambda)$$

$$= F(C_{m+t-1}, \lambda) F(C_{n+t-1}, \lambda) + F(C_{m+n-2t+2}, \lambda).$$

By above argument the proof is completed. ▀
**Theorem 2.** Let $G$ be a simple graph with edge disjoint cycles without bridge edge. Then the flow polynomial of $G$ is obtained as follows:

$$F(G, \lambda) = (\lambda - 1)^t.$$ 

where $t$ is the number of cycles of $G$.

**Proof.** Apply Theorems C and D. □

**Corollary 3.** Let $D$ be a dendrimer with a bridge edge then $F(G, \lambda) = 0$.

**Proof.** Apply Theorems F. □

**References**