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ON SOME EXTENSIONS OF MURRAY'S LAW

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Abstract: This paper cites the original Murray's law about optimal radii. Extensions to some class of non-Newtonian flows that are described by the Ostwald-de Waele model and the Newtonian flows for elliptical cross-sections. A generalisation of Murray's law for multi-objective formulation is also given. It is shown that the original formulation of the optimal condition is a particular case of the multi-objective formulation.

Keywords: fluid mechanics, bioflows

Notation

a, b – ellipse semi-axes,
A, B, C – constants,
f, $\boldsymbol{f}$, f_i – functions,
$\boldsymbol{g}$ – target vector,
H – Hessian,
k – consistency constant,
L – length of an artery,
n – rheological parameter, number of objective functions,
m – metabolic coefficient, space dimension,
N, N_d, N_m – total, dissipation and metabolic power,
N^+ – dimensionless power,
$\boldsymbol{N}$ – vector of objective functions,
$\mathbb{N}$ – natural number set,
$\mathscr{N}$ – natural number subset,
$\mathscr{P}$ – Pareto set front,
$\mathbb{R}$ – real number set,
R – radius,
V – artery volume,
$\dot{V}$ – volume flow rate,
w_i, $\boldsymbol{w}$, $\boldsymbol{W}$ – weights, vector and matrix of weights,
$\boldsymbol{x}$, x_i – points (solutions),

γ – shear rate, second invariant,
$\boldsymbol{\delta}$ – Kronecker delta,
Δp – pressure drop,
λ – weight,
μ – molecular viscosity coefficient,
Π – Pareto set,
Ω – admissible solutions set.

1. Introduction

The two Murray's laws [1, 2] describe the pattern of large to small or conversely small to large artery bifurcation. This is due to the optimal configuration of arteries that allows for fastest transport with minimal work involved. Murray's laws are valid for the tree structure of arteries, see Figure 1.

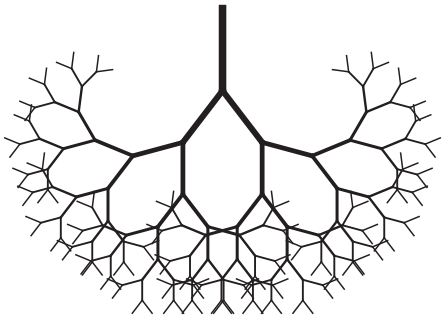

Figure 1. Tree structure

One of Murray's laws gives a formula for the radii, whereas the second law specifies the angles of bifurcation. Both laws were formulated for arteries but they are not limited to this venue. Some technical applications also exist [3]. The original Murray's law about radii [2] was derived only for Newtonian fluids, for circular cross-sections of arteries. Single criterion minimisation methods were also used for the derivation. A generalisation of Murray's law for multi-objective formulation is given here to some non-Newtonian and Newtonian fluids within elliptical cross-sections. It is shown that the original formulation of the optimal condition is a particular case of multi-objective formulation.

2. Murray's law about optimal radii

The original Murray's reasoning [2] takes into consideration two energy terms that contribute to maintaining the blood flow. These are the energy necessary for overcoming the viscous drag (dissipation energy) and the metabolic power necessary for maintaining the volume of blood within an artery. For steady state flows it is more convenient to use dissipation power N instead of energy E. These quantities are explicitly related as $E = \int_0^t N \,\mathrm{dt} = N t$. The dissipation power is given by $N_d = \dot{V} \Delta p$. By means of Hagen-Poiseuille's law [4] and the definition of constant $A := 8\mu L \pi^{-1}$ it is possible to express this power as $N_d = A \dot{V}^2 R^{-4}$.

The metabolic power is expressed as $N_m = mV$ where m is a metabolic coefficient and volume V is given by $V = \pi R^2 L$. Introducing another constant $B := \pi L m$ we can rewrite the metabolic power N_m in the following form $N_m = BR^2$.

The equation for N_d suggests that dissipation power N_d is related inversely, and metabolic power N_m directly, to radius R. It suggests that there exists an intermediate radius which minimises the total power $N = N_d + N_m$. This total power may be expressed as $N = A\dot{V}^2 R^{-4} + BR^2$. For a given $\dot{V}$ the total power N is a function of R. The stationary point can be found from the condition $N'(R) = 0$ which gives $R = \dot{V}^{1/3} C^{-1/3}$ or

$$\dot{V} = CR^3 \tag{1}$$

where constant C is combined of A and B as $C := 2^{-1/2} A^{-1/2} B^{1/2}$. The sign of the second derivative is $N''(\dot{V}^{1/3} C^{-1/3}) = 12B \geq 0$. This is because A and B are positive. The solution (1) represents a constant relation between the volumetric flow rate and the radius in every cross-section of an artery. This is also a condition for minimal energy requirement.

The mass conservation equation gives us information that the flow rate before any bifurcation equals the sum of individual flow rates after that bifurcation $\dot{V}_0 = \sum_i \dot{V}_i = CR_0^3$. This is true for incompressible and steady state flows. Equation (1) allows us to write $\sum_i \dot{V}_i = C \sum_i R_i^3$. This is true because before and after bifurcation we deal with the same fluid which means that we have the same constant C. The above two equations give us Murray's law which states that the cube of the radius of the parent artery equals the sum of the cubes of the radii of the daughter arteries. This is written as:

$$R_0^3 = \sum_i R_i^3 \tag{2}$$

In the case of bifurcation this simplifies to $R_0^3 = R_1^3 + R_2^3$. It is the most widespread form of Murray's law and it is known that a large part of the branching of the mammalian circulatory and respiratory systems obeys it [3]. Some experimental comparisons are given [3, 5].

Assuming that Murray's law is valid it is possible to evaluate the metabolic coefficient m. Using the definitions of A, B and C one can show that this coefficient may be written as $m = 16\pi^{-2} \mu C^2$. Since Equation (1) is valid for every branch it allows us to determine the value of constant C. Eventually, the metabolic coefficient is given by means of the following equation:

$$m = \frac{16\mu \dot{V}^2}{\pi^2 R^6} \tag{3}$$

3. Non-Newtonian flow

3.1. The Ostwald-de Waele model

In the Ostwald-de Waele model (power law) [6] molecular viscosity is a function of shear rate γ. For simple shear flows it is:

$$\mu = k|\gamma|^{n-1} \tag{4}$$

For three dimensional flows γ is related to the second invariant of strain rate tensor [7]. The mechanical constitutive equation that expresses viscosity as a function of γ belongs to the generalised Newtonian constitutive equation. In spite of the name these flows are non-Newtonian. The greater the dimensionless rheological parameter, n, present in Equation (4), the greater the non-Newtonian flow behaviour. The greater the consistency index, k, the more viscous the flow is. For $n := 1$ and $k \equiv \mu$ we have Newtonian viscosity. Equation (4) makes it possible to model the shear-thinning behaviour ($n < 1$) and shear-thickening ($n > 1$). The Ostwald-de Waele model is the simplest non-Newtonian model and due to this is very useful as well as capable of blood flow approximation. The volume flow rate for cylindrical cross-sections may be calculated as:

$$\dot{V} = \frac{n\pi R^{3+\frac{1}{n}}}{1+3n}\left(\frac{\Delta p}{2kL}\right)^{\frac{1}{n}} \tag{5}$$

and is a generalisation of Hagen-Poiseuille's law for the Ostwald-de Waele's model.

3.2. Murray's law form

Following the same logic as in paragraph 2 it may be shown that for the non-Newtonian case described by the Ostwald-de Waele model we obtain exactly the same form of Murray's law. It is enough to take advantage of formulae $N_d = \dot{V}\Delta p$ and (5). The dissipation power takes the form:

$$N_d = 2kL\left(\frac{1+3n}{n\pi}\right)^n \frac{\dot{V}^{n+1}}{R^{3n+1}} = A\frac{\dot{V}^{n+1}}{R^{3n+1}} \tag{6}$$

A new definition of constant A follows from the above equation. The metabolic power remains the same as previously. The necessary condition for the extreme gives us:

$$\dot{V} = \left(\frac{2B}{(3n+1)A}\right)^{\frac{1}{n+1}} R^3 = CR^3 \tag{7}$$

The form of this equation is identical as previously for the Newtonian case (1). The only difference is the definition of the constant C. For $n = 1$ everything is reduced to the Newtonian case.

4. Flows in elliptical channels

4.1. Solution for elliptical cross-section

It can be shown that in generalised cylindrical coordinates it is not possible to integrate the differential equations of the motion. This case differs from the cylindrical one. However, this difficulty can be overcome by approximate methods. The Ritz method [4] is one of the possibilities. It even gives an exact solution for the case of an elliptical cross-section. Taking advantage of such a solution for velocity field [4] it is possible to determine the volumetric flow rate in the form:

$$\dot{V} = \frac{\Delta p a^3 b^3 \pi}{4\mu L(a^2+b^2)} \tag{8}$$

For $a = b = R$ Equation (8) simplifies to the cylindrical case.

4.2. Murray's law form

Murray's law preserves its validity for elliptical cross-sections. If we take $N_d = \dot{V}\Delta p$ and Equation (8) the dissipation power yields:

$$N_d = \dot{V}^2 A \frac{a^2+b^2}{a^3 b^3} \tag{9}$$

where constant A equals $A := 4\mu L\pi^{-1}$. Metabolic power $N_m = m\pi abL = Bab$ remains intact. The total power $N = N_d + N_m$ depends on the two variables, a and b. The stationary point may be found as a solution of the two equations, $\frac{\partial N}{\partial a} = 0$ and $\frac{\partial N}{\partial b} = 0$. It follows that $a = b = R = \dot{V}^{1/3}(2A/B)^{1/6}$. This means that the ellipse should take the form of a cylinder to minimise the total power. The first sufficient condition requires the Hessian:

$$H(a,b) = \begin{vmatrix} \frac{\partial^2 N}{\partial a^2} & \frac{\partial^2 N}{\partial a \partial b} \\ \frac{\partial^2 N}{\partial a \partial b} & \frac{\partial^2 N}{\partial b^2} \end{vmatrix} \tag{10}$$

to be positive. This condition is satisfied. This is because $H(R,R) = 33B^2 > 0$. The second sufficient condition (for minimum) is also satisfied $\frac{\partial^2}{\partial a^2} N(R,R) = 7B > 0$. Finally, we have the well known formula $\dot{V} = CR^3$ where C is of similar form as previously $C := 2^{-1/2} A^{-1/2} B^{1/2}$. The only difference is the definition of the constant A.

5. Multi-objective description of Murray's law

Since the Murray reasoning takes into consideration two powers (objective functions) it is then a natural multi-objective optimisation problem. A whole set of optimal solutions known as the Pareto set is obtained as a solution of such a problem. There is also a number of scalarisation methods of the multi-objective problem. They are very useful because they allow obtaining a Pareto set by means of single objective optimisation methods. The problem considered by Murray (sum of two powers) is just one particular scalarisation method.

5.1. Basic information

Vector $\boldsymbol{f}$ of n scalar functions f_i is denoted as $\boldsymbol{f} := (f_1, \ldots, f_n)$. If a point (solution) $\boldsymbol{x}$ in m-dimensional space $\mathbb{R}^m$ is denoted by $\boldsymbol{x} := (x_1, \ldots, x_m)$ then the n-dimensional objective fitness function value is $\boldsymbol{f}(\boldsymbol{x}) := (f_1(\boldsymbol{x}), \ldots, f_n(\boldsymbol{x}))$. From this it follows that the function $\boldsymbol{f}$ maps from m- to n-dimensional space $\boldsymbol{f} : \mathbb{R}^m \to \mathbb{R}^n$. Individual fitness functions f_i, being components of $\boldsymbol{f}$, map $f_i : \mathbb{R}^m \to \mathbb{R}$. Let us also introduce a subset $\mathscr{N}$ of a set of natural numbers $\mathscr{N} := \{1, \ldots, n\} \subseteq \mathbb{N}$ of n numbers.

Domination is a key concept for multi-objective optimisation. In the case of minimisation of function $\boldsymbol{f}$ it is assumed that point $\boldsymbol{x}_1$ dominates over point (or solution) $\boldsymbol{x}_2$ if $\forall_{i \in \mathscr{N}} f_i(\boldsymbol{x}_1) \leq f_i(\boldsymbol{x}_2) \wedge \exists_{i \in \mathscr{N}} f_i(\boldsymbol{x}_1) < f_i(\boldsymbol{x}_2)$ where $\boldsymbol{x}_1, \boldsymbol{x}_2 \in \Omega \subseteq \mathbb{R}^m$. Here the set of all admissible solutions is denoted as Ω. When we deal with a maximisation of function $\boldsymbol{f}$ then one has to exchange relations $\leq$ and $<$ in the above definition with $\geq$ and $>$, respectively. We can say, by contradiction

of definition, that $\boldsymbol{x}_1$ does not dominate (for minimisation) over $\boldsymbol{x}_2$ (or $\boldsymbol{x}_2$ is not dominated by $\boldsymbol{x}_1$) if $\exists_{i\in\mathscr{N}} f_i(\boldsymbol{x}_1) > f_i(\boldsymbol{x}_2) \vee \forall_{i\in\mathscr{N}} f_i(\boldsymbol{x}_1) \geq f_i(\boldsymbol{x}_2)$. Hence, the Pareto set Π of the solution is a set of those points which are not dominated by others from the set of admissible solutions Ω. This can be denoted as:

$$\Pi := \left\{ \boldsymbol{x}_j \in \Omega : \underset{\boldsymbol{x}\in\Omega}{\forall} \Big(\underset{i\in\mathscr{N}}{\exists} f_i(\boldsymbol{x}) > f_i(\boldsymbol{x}_j) \ \vee \underset{i\in\mathscr{N}}{\forall} f_i(\boldsymbol{x}) \geq f_i(\boldsymbol{x}_j) \Big) \right\} \tag{11}$$

A more detailed discussion on the multi-objective optimisation is given in [8].

5.2. Typical scalarisation methods

Multi-objective optimisation gives a whole set of optimal solutions whereas a single value of power is needed. There is a need for choosing one solution from the Ω set. There are two ways. One can choose this solution directly from the Ω when the multi-objective optimisation is finished or to solve a single objective optimisation problem from the beginning instead. The latter needs scalarisation vector $\boldsymbol{f} : \mathbb{R}^m \to \mathbb{R}^n$ to single $f : \mathbb{R}^m \to \mathbb{R}$.

The most popular method is the weighted-sum method. The n-dimensional vector of weights $\boldsymbol{w} := (w_1, \ldots, w_n)$ is composed of individual weights $w_i \in [0,1]$ which can be optionally selected, provided that $\sum_{i=1}^{n} w_i = 1$. The values of individual weights represent the importance of a given function f_i. Function f is obtained from $\boldsymbol{f}$ by the dot product of function $\boldsymbol{f}$ and vector of weights $\boldsymbol{w}$ in the form of $f(\boldsymbol{x}) := \boldsymbol{w} \cdot \boldsymbol{f}(\boldsymbol{x}) = \sum_{i=1}^{n} w_i f_i(\boldsymbol{x})$. A proper selection of weights produces convergence for individual elements of the Pareto set.

Apart from the weighted-sum method there is also target vector $\boldsymbol{g}$. This method reduces the function $\boldsymbol{f}$ to f by means of $f(\boldsymbol{x}) := \|(\boldsymbol{f}(\boldsymbol{x}) - \boldsymbol{g}) \cdot \boldsymbol{W}^{-1}\|_\alpha$. Symbol $\boldsymbol{W}$ represents a matrix of weights and it is usually the diagonal of size $n \times n$. Vector $\boldsymbol{g}$ represents imaginary optimal values to which an algorithms tries to converge. For the target vector method the norm $\|\cdot\|_\alpha$ is replaced by the generalised Euclidean norm in the form $\|\boldsymbol{a}\|_\alpha := (\sum_{i=1}^{n} |a_i|^\alpha)^{1/\alpha}$. Usually $\alpha := 2$ and $\boldsymbol{W} := \boldsymbol{\delta}$ where $\boldsymbol{\delta}$ represents the Kronecker delta.

5.3. Murray's law form

A simultaneous optimisation of two powers (objective functions) in the form $\boldsymbol{N} := (N_d, N_m)$ results in a non-dominated set of solutions (Pareto set). It is possible to obtain an analytical solution describing the so called Pareto front $\mathscr{P}$. Taking advantage of the weighted-sum method we can obtain a parametric representation of the solution where λ is a parameter. The scalarised form of the objective function is obtained as $N := \boldsymbol{w} \cdot \boldsymbol{N}$ and takes the shape of $N := \lambda N_d + (1-\lambda) N_m$. The necessary condition for extreme $N'(R) = 0$ gives us a formula which is analogous to (1):

$$\dot{V} = \left(\lambda^{-1} - 1\right) C R^3 \tag{12}$$

According to Murray the dissipation power, N_d, and the metabolic power, N_m, have identical contribution in the total power, N. This corresponds to

a situation where the weight in Equation (12) equals $\lambda = 2^{-1}$. In the multi-objective description it means that both powers are equally important. However, it follows from Equation (12) that it does not have to be so. If we incorporate Equation (12) into mass conservation equation $\dot{V}_0 = \sum_i \dot{V}_i$ we obtain the well known form of Murray's law (2). This means that one of the powers can have a larger share than the other. A 'share' means weights λ and $1-\lambda$ for any $\lambda \in]0;1[$. The above reasoning generalises Murray's law.

Radius R may be found from Equation (12) and incorporated into equations $N_d = A\dot{V}^2 R^{-4}$ i $N_m = BR^2$. Rearranging and introducing the dimensionless powers N_d^+, N_m^+ we have:

$$N_d^+ := \frac{N_d}{(AB^2\dot{V}^2)^{\frac{1}{3}}} = 2^{-\frac{2}{3}} \left(\lambda^{-1} - 1\right)^{\frac{4}{3}} \tag{13a}$$

$$N_m^+ := \frac{N_m}{(AB^2\dot{V}^2)^{\frac{1}{3}}} = 2^{\frac{1}{3}} \left(\lambda^{-1} - 1\right)^{-\frac{2}{3}} \tag{13b}$$

The Pareto front $\mathscr{P}$ takes the following form:

$$\mathscr{P} = \left\{ (N_d^+, N_m^+) : N_d^+ := 2^{-\frac{2}{3}} \left(\lambda^{-1} - 1\right)^{\frac{4}{3}}, \; N_m^+ := 2^{\frac{1}{3}} \left(\lambda^{-1} - 1\right)^{-\frac{2}{3}} \right\} \tag{14}$$

A formal definition of the Pareto front is that it is a set of points with coordinates corresponding to Pareto set elements. It is written as $\mathscr{P} := \{\boldsymbol{f}(\boldsymbol{x}) : \boldsymbol{x} \in \Pi\}$. The Pareto front is shown in Figure 2. The point with weight $\lambda = 2^{-1}$ is marked.

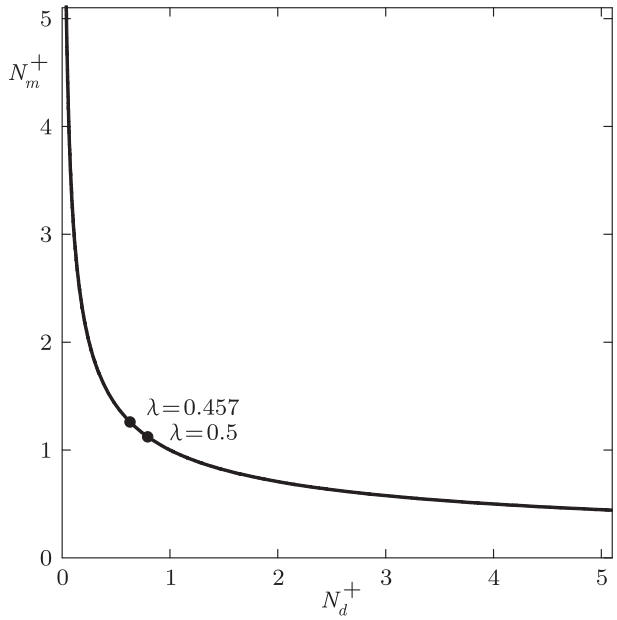

Figure 2. The Pareto front $\mathscr{P}$

Instead of choosing a solution that treats both powers as equally important ($\lambda = 2^{-1}$) it is also possible to apply the target vector method. The target vector is chosen as an imaginary optimum. A natural choice for this optimum is such a vector for which both powers equal zero. This is really an imaginary vector because the dissipation power for viscous flows does not equal zero [4]. However, it is assumed that the target vector $\boldsymbol{g} = (0,0)$. The vector is localised in the centre of the coordinate system in Figure 2. According to discussion in paragraph 5.2 the scalarisation $\boldsymbol{N}$ to N is done by means of norm $N := \|\boldsymbol{N} - \boldsymbol{g}\|_2$ because $\boldsymbol{W} := \boldsymbol{\delta}$. The norm $\|\cdot\|_2$ is just Euclidian norm $N = (N_d^2 + N_m^2)^{1/2}$. It is assumed that the target vector $\boldsymbol{g} = \boldsymbol{0}$ simplifies also the calculations. The necessary condition for extreme $N'(R) = 0$ gives a similar equation to (12):

$$\dot{V} = 2^{\frac{1}{4}} C R^3 \tag{15}$$

The weight of this solution equals $\lambda \approx 0.457$ and is shown in Figure 2. What is interesting, the point (N_d^+, N_m^+) for this weight is not placed closer to the target vector (0,0). This is because the Pareto front converges 'faster' to its own vertical asymptote rather than to the horizontal one. It is well visible in Figure 2. Again, using the formula (15) and the mass conservation equation, it is possible to show that Murray's law takes the standard form (2). What is more, one can observe that the solution (15) obtained by means of the target-vector method is another particular case of that obtained by means of weighted sum method (12). The same concerns the original Murray's solution for which $\lambda = 2^{-1}$.

6. Conclusions

Murray's law for artery radii is valid for non-Newtonian fluids described by means of the Ostwald-de Waele model. For the case of elliptical cross-sections the minimal total power is obtained for the cylindrical shape. The multi-objective formulation of Murray's law makes it possible to generalise it. It is not necessary for both powers to be equally important. Other cases are possible in the sense of weights. The original minimal energy requirement condition $\dot{V} = CR^3$ is a particular case where the weight $\lambda = 2^{-1}$. Another particular case comes from the target-vector method where $\lambda = 2^{1/4}$. This method, however, does not assume that both powers are equally important. It converges to the imaginary optimum instead.

Further simplifications allow achieving interesting estimates by means of Murray's law. For the case of symmetrical bifurcations ($R_1 = R_2$) Murray's law simplifies to $R_0/R_1 = 2^{1/3}$. For the subsequent bifurcation we have $R_1/R_2 = 2^{1/3}$. Generally speaking, $R_0/R_m = 2^{m/3}$. This allows finding the bifurcation number m as a function of the radii ratio of the first and last artery:

$$m = \frac{\ln \frac{R_0}{R_n}}{\ln 2^{\frac{1}{3}}} \tag{16}$$

Knowing the aorta and capillary ratio (*e.g.* $R_0/R_m = 1500$) it is possible to estimate the optimal number of bifurcations from the aorta to capillaries which

is about 31. By means of the same assumptions we can estimate that there are a few billion of capillaries (2^m). Actually, there are more. This is because we have a branching which varies from symmetric bifurcation. Additionally, below a certain dimension or radii the tree structure becomes a network structure [5].

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