Extending the System Dynamics Toolbox to Address Policy Problems in Transportation and Health

By

Nasim Seyed Zadeh Sabounchi

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Hazhir Rahmandad, Chair
Konstantinos P. Triantis, Co-Chair
G. Don Taylor
Sudipta Sarangi

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ABSTRACT

System dynamics can be a very useful tool to expand the boundaries of one's mental models to better understand the underlying behavior of systems. But despite its utility, there remains challenges associated with system dynamics modeling that the current research addresses by expanding the system dynamics modeling toolbox. The first challenge relates to imprecision or vagueness, for example, with respect to human perception and linguistic variables. The most common approach is to use table or graph functions to capture the inherent vagueness in these linguistic (qualitative) variables. Yet, combining two or more table functions may lead to further complexity and, moreover, increased difficulty when analyzing the resulting behavior. As part of this research, we extend the system dynamics toolbox by applying fuzzy logic. Then, we select a problem of congestion pricing in mitigating traffic congestion to verify the effectiveness of our integration of fuzzy logic into system dynamics modeling.

Another challenge, in system dynamics modeling, is defining proper equations to predict variables based on numerous studies. In particular, we focus on published equations in models for energy balance and weight change of individuals. For these models there is a need to define a single robust prediction equation for Basal Metabolic Rate (BMR), which is an element of the energy expenditure of the body. In our approach, we perform an extensive literature review to explore the relationship between BMR and different factors including age, body composition, gender, and ethnicity. We find that there are many equations used to estimate BMR, especially for different demographic groups. Further, we find that these equations use different independent variables and, in a few cases, generate inconsistent conclusions. It follows then that selecting a single equation for BMI can be quite difficult for purposes of modeling in a systems dynamics context. Our approach involves conducting a meta-regression to summarize the available prediction equations and identifying the most appropriate model for predicting BMR for different sub-populations. The results of this research potentially could lead to more precise predictions of body weight and enhanced policy interventions to help mitigate serious health issues such as obesity

Dedication

This work is dedicated to my lovely parents Seyed Javad and Nahideh, and my beautiful sisters Shabnam and Sepideh, without whose caring support it would not have been possible, and to the memory of my grandparents, Mirnazir and Iran.

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1. Introduction

System Dynamics can be effective to "expand the boundaries of our mental models, enhance our ability to generate and learn from evidence, and catalyze effective change" (Sterman, 2006, p. 505). There are challenges associated with system dynamics modeling that this research addresses by expanding the system dynamics modeling toolbox. One challenge is related to dealing with imprecision or vagueness, for example in respect to human perception and linguistic variables. Another challenge, relates to defining equations to better predict variables based on numerous studies.

In regards to dealing with imprecision, the most common approach in the literature is to use table or graph functions to capture the inherent vagueness in linguistic variables. However, combining two or more table functions creates further complexity and often is not easy to analyze the resulting behavior. In this research, we broaden the use of system dynamics modeling by applying the fuzzy logic approach. We select as an example results for an application to the problem of traffic demand management. Additionally, in systems dynamics modeling there is a need for defining robust equations for variables. As an example, we study the case of finding robust equations in the literature for predicting Basal Metabolic Rate (BMR), an element of energy expenditure of the human body. We find that after an exhaustive literature review and meta-analysis that we are able to summarize the available prediction equations used to define a single structure or model.

2. Research Strategy

The body of this research project has been organized into three essays. The first essay attempts to bridge fuzzy logic and system dynamics to enhance the ability of dealing with vagueness inherent in for example linguistic variables. The second essay focuses on applying the methodology described and justified in the first essay to a real world application of implementing a congestion pricing scheme in a cordon based area. In this application, study participant's perceptions regarding the congestion level and cost of driving, plus the metro service level are deemed vague and riddled with uncertainty lending them for application of the fuzzy logic approach. In the last essay, in searching for the most appropriate model for predicting Basal Metabolic Rate (BMR) for different sup-populations and demographic groups, we perform a comprehensive review of published works in the health domain. Next, we conduct a meta-regression and find the robust prediction equations. What follows is a short description of the three essays as well as how each contributes to the core research question and to the attainment of the objectives of this research.

The first essay, "Challenges and Insights Associated with Fuzzy Modeling in a System Dynamics Context", builds on the method developed by Liu, Triantis, and Sarangi (2010b) wherein a fuzzy logic approach incorporates linguistic variables for dynamic modeling. Because the implementation of fuzzy logic in system dynamics is not straightforward especially for multiple linguistic variables, a number of challenges follow. First, there is no unique fuzzification and defuzzification method that can be used since each method has its own inherent strengths and weaknesses. Second, fuzzy logic requires definition of consistent fuzzy rules, which is not a straightforward task. Further, the overall use of fuzzy logic is not easy for the use of one let alone the use of several linguistic variables. And finally, the interpretation and the validity of the results obtained from this research remains a key issue. The major contribution of this essay is the array of insights revealed in addressing these challenges.

An exhaustive exploration of all possible issues would be well beyond the scope of a single research paper, and so we narrow our purview to the problem of selecting a particular set of the fuzzy rules (e.g., a combination of optimistic and pessimistic approach) and the Max-Min fuzzy inference mechanism. We then study the implications of using each de-fuzzification method prescribed by the approach proposed by Liu et al. (2010b). To facilitate a polar case comparison, we adopt the Largest of the Maximum (LOM) and Center of Area (COA) defuzzification methods. Based on our analysis, we highlight various interpretations and modeling challenges associated with each and assess any departures from the norm in applying fuzzy logic reasoning.

In the second essay, "Simulation Modeling and Policy Analysis for Evaluating the Dynamic Impacts of a Congestion Pricing Policy for a Transportation Socioeconomic System", we create a system dynamics model based on the framework established by Liu, Triantis and Sarangi (2010a), for evaluating the impact of congestion pricing policy on mitigating the traffic congestion in a cordon based area. The main objective of the congestion pricing scheme is to improve alternative transportation modes by distributing part of the revenues generated by the scheme. This allocation serves to mitigate traffic congestion and the negative effects of traffic congestion on people's lives. The major consideration in developing the model is that congestion, cost of driving, and the supply and demand associated with mass transit affect individual behavior.

In our approach, we address the persistent issue of multiple linguistic variables which are a natural consequence when dealing with human subjects. These variables cannot be easily quantified because they are manifested in natural or artificial language. We employ the use of linguistic variables to represent human perceptions of travel modes. Three separate linguistic variables capture perception wherein fuzzy set theory evaluates the combined effect of the perception values. In particular, perceptions of travel mode selection and switching behavior between travel modes. The integration and operation of multiple linguistic variables in a system dynamics framework, provides an alternative means to represent behavioral variables in social system modeling. In this regard, we answer the call of the first essay for applying fuzzy logic.

To verify the effectiveness of congestion pricing policy, a system dynamics model simulates revenues generated from the scheme and their impact on transportation modes and the effectiveness of mitigating traffic congestion caused by material and information delays. The model calibration against data based on a pricing scheme for the London (U.K.) cordon. Overall, the developed model can be used to evaluate various travel demand management strategies and/or combinations of strategies. Consequently, we can determine proper policies and best cases for critical parameters leading to the discovery of optimum results in terms of implementing a particular pricing scheme.

Finally the third essay, “Basal Metabolic Rate: Systematic Review and Meta-Regression for Proposing General Prediction Equations”, we present body weight dynamics in a more precise manner as we employ a novel methodology for a single robust equation for Basal Metabolic Rate of the human body. Current dynamic energy balance models define the Basal Metabolic Rate (BMR) as a constant value, which constitutes a significant portion of total energy expenditure of the body (Rahmandad & Sabounchi, 2011). Based on the overview of the literature, there are several equations that estimate the BMR for different demographic groups, using the same or different structural forms. These equations use different independent variables and come to somewhat inconsistent conclusions in a few cases. This fact motivated us to perform a comprehensive systematic review and conduct a meta-regression analysis to find the most appropriate model for predicting BMR for different sup-populations and demographic groups. The results of this research could potentially be used in studying the dynamics and feedback between BMR and related factors so that BMR can also be included as an endogenous variable in a model of predicting body weight dynamics. Furthermore, we leave as an open research question the development of more precise predictions of BMR that potentially could lead to more robust policy intervention to mitigate the increase in obesity.

The three essays, outlined above, are related to each other by addressing two specific needs identified in the literature. First, the need to model linguistic (qualitative) variables in a system dynamics modeling context by using the fuzzy logic approach. This leads to further capability, especially when dealing with multiple linguistic variables Second, the affinity for a comprehensive literature search and compilation of the numerous studies that all in one way or another attempt to estimate dependent variables based on macro independent variables. Our results lead to more precise predictions robust policy intervention analysis in traffic congestion and health domains. In conclusion, this dissertation expands the system dynamics toolbox by bridging to fuzzy logic for linguistic variables and by poising equations from a health context for integration into future systems dynamics modeling.

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First Essay:

Challenges and Insights Associated with Fuzzy Modeling in a System Dynamics Context

Abstract

In this paper, we build on a previously proposed approach to bridge fuzzy logic with dynamic modeling, by incorporating linguistic variables in a system dynamics context. The motivation for this approach is to illustrate how to combine vague dynamic variables in a meaningful way. Several challenges follow immediately including the selection of the fuzzification and defuzzification method, the implementation in a system dynamics framework and assessing the validity of the results. For illustrative purposes we use a variant of a sales and service model. This model is based on the concepts of product diffusion, backlog accumulation and personnel adjustments and their respective existing modeling representations in the literature. We focus on certain popular membership functions, and apply the max-min fuzzy inference approach as a way to combine two or more fuzzy variables. Then we summarize the joint effect of the linguistic variables by applying two defuzzification methods (largest of maximum and center of area). This allows us to highlight various interpretation and modeling challenges associated with each defuzzification method and the applied inference mechanism. Based on our results, the utilization of either defuzzification method leads to some counterintuitive results. We then suggest modifying the fuzzy inference method, in order to make the defuzzified values behave reasonably.

Key Words and Phrases: System Dynamics, Fuzzy Sets, Linguistic variables, Uncertainty, Defuzzification

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1. Introduction

Modeling linguistic variables often leads to situations that are fraught with uncertainty and are difficult to quantify. One typically encounters two separate issues. The first deals with the ambiguity that surrounds the linguistic variable in question which is best described by the lack of information about the variable itself. The second issue arises from the way the uncertain variable is described (Kikuchi, 2005).

The latter aspect of uncertainty is the focus of this paper since researchers wish to ensure that relevant variable characteristics along with the way they are perceived (or measured) have been accurately captured. For instance, the perception of the Level of Service (LOS) concept is often best expressed in linguistic terms by various gradual states such as, very good, good, not good, etc. and it is very difficult to accurately capture these different states of perception in a quantitative manner. Furthermore, measuring how this variable changes over time poses an additional challenge since one would wish to have a reasonable representation of the changes of the state of the uncertain variable through time. Consequently, it is important to investigate the feasibility and issues that arise when using a fuzzy logic based representation of linguistic variables in a dynamic modeling context.

For static representations or problems, fuzzy logic has been proposed as an approach to deal with aspects of vagueness typically expressed in linguistic terms (Kikuchi, 2005). Hence, our motivation arises from the possibility of capitalizing on the modeling strengths associated with the fuzzy logic approach especially when one is dealing with multiple linguistic variables in a dynamic context. As highlighted in the next section, this research addresses two specific needs identified in literature: (*i*) the need to explicitly model linguistic (qualitative) variables in a dynamic modeling context using alternative formulations, and (*ii*) the need to explicitly consider dynamic behavior when considering a fuzzy reasoning framework. The approach taken in this paper is an alternative approach to the most common one taken in system dynamics modeling, which is to use table or graph functions to capture the inherent vagueness of linguistic variables (Ford & Sterman, 1998).

This paper builds on the method developed by Liu, Triantis, and Sarangi (2010) where a fuzzy logic approach was proposed as a way to incorporate linguistic variables in dynamic modeling. The motivation for this research paper originated in part by the implementation and interpretation difficulties associated with the use of the largest of maximum de-fuzzification method within a fuzzy logic inference approach where the dynamic consequences of congestion pricing were studied (Liu, 2007). This naturally has led to the question of how other de-fuzzification methods would perform in a similar dynamic modeling context. A number of challenges follow immediately. First, there is no unique fuzzification and defuzzification method that can be used since each has its own strengths and weaknesses. Second, the actual implementation of this fuzzy logic approach in a system dynamics framework is not trivial especially when one wishes to incorporate multiple linguistic variables. Finally, the interpretation and the validity of the results obtained from this approach remains a key issue. As we show below these different issues can be inter-related and hence cannot be dealt with in isolation.

However, an exhaustive exploration of all of these issues and a complete solution to this general problem is beyond the scope of a single paper. Our goal and contribution is to discuss the issues and provide the initial useful insights associated with this general problem and to suggest ways to deal with these challenges. In this paper, we analyze the problem by only considering a certain set of the fuzzy rules (the combination of an optimistic and pessimistic approach) and the Mamdani (1977) fuzzy inference mechanism. Then we study the implications of using the two alternative de-fuzzification methods within the approach proposed by Liu, et al. (2010). To facilitate a comparison, two different defuzzification methods are applied in the model, i.e., the 'Largest of the Maximum (LOM)' and the 'Center of Area (COA)'.[1] The fuzzification method and fuzzy rules are kept the same for the different de-fuzzification methods. Based on our analysis, we highlight various interpretation and modeling challenges associated with each de-fuzzification method in a system dynamics modeling context and examine the results when we are applying the fuzzy reasoning framework.

In our earlier work (Sabounchi, Triantis, Sarangi, & Liu, 2011), the issues and challenges are introduced, but a complete analysis is not provided. In this paper, a detailed analysis is detailed that illustrates the resulting behavior associated with the interaction between different linguistic variables. Although studies have been done in the past to analyze both the effect of the various types of inference and defuzzification methods (Butkiewicz, 2004; Gupta & Qi, 1991; Mizumoto, 1989, 1995; Saade, 1996), our objective is different from this existing literature since we incorporate fuzzy logic modeling into a system dynamics context and hence the need for defuzzification is different.

The essence of the methodological approach adopted in this paper requires (1) the definition of membership functions as representations of the degree to which specific variable attributes hold, (2) the application of Mamdani's (1977) max-min direct inference approach as a way to combine two or more fuzzy variables, and (3) the use of two de-fuzzification approaches (largest of maximum and center of area) that capture (summarize) the joint effect of the linguistic variables. For illustrative purposes we use a variant of a sales and service model described by Liu, et al. (2010), which is based on the concepts of product diffusion, backlog accumulation and personnel adjustments and their respective existing modeling representations in the literature (Hines, 2004).

As is well known in the literature (J. Sterman, 2000), the product diffusion model is about introducing a new product in the market. The growth of the market share depends upon the attractiveness of the product among potential customers and a favorable word of mouth that makes more potential customers buy the product. The conversion of non-customers to customers, is related to product attractiveness making it the driving force in such models. There

[1] In the literature sometimes the term 'Center Of Gravity (COG)' is used, even though it is computed only for a two-dimensional area.

are several factors that determine product attractiveness including for example 'delivery timeliness' and 'customer service' available for the product.

However, the perceptions with respect to 'delivery timeliness' and 'customer service' have an inherent vagueness that makes a precise or crisp representation difficult. In other words, in the proposition "Customer Service is Satisfactory", the premise 'customer service' can be estimated with certainty based on measured values that hold. However, the consequent satisfaction level is typically vague. For example, if a measured representation of customer service ranges between zero and one and if this value is 0.9, it is reasonable to assume that the perception regarding customer service would most possibly be viewed as high, but 'high' itself is a relative term and hence has a vague definition. Altogether, we can describe the perceptions of customers in linguistic terms such as low, medium and high, which all have vague definitions. Furthermore, these perceptions change over time especially since there are forces at work (e.g., the training of the sales force) that can affect these perceptions. Hence, the representation of perceptions such as these over time provides the key motivation for exploring the fuzzy logic concepts in the context of dynamic modeling.

This paper is structured as follows. Section 2 provides a brief literature review on applying fuzzy logic in the system dynamics modeling paradigm. Then in Section 3, the model that is used for illustrative purposes is explained in detail. In Section 4, the fuzzification process and the inference method used in the developed model is described. The results from the two defuzzification approaches including the Largest of Maximum (LOM) and Center of Area (COA) approaches are studied thoroughly in Section 5. Some counter-intuitive results are also highlighted in this section. A comprehensive comparison of results from the two defuzzification approaches is provided in Section 6. Finally, in Section 7, we conclude with a summary of the main results along with recommendations for future research.

2. Background

There have been several attempts to bridge fuzzy logic with dynamic modeling. Levary (1990) suggests that if the system dynamics methodology is extended to deal with imprecision or vagueness, then it would be more effective in modeling real-life systems and proposes applying the concept of fuzzy sets introduced by Zadeh (1965), but, the author does not actually implement the suggestions in an actual system dynamics model.

Maeda, Asaoka, and Murakami (1996) point out that fuzzy reasoning methods, "… have not dealt with the notion of time and have not provided a means for utilizing a time delay between premise and consequent." (p. 101). They propose a reasoning method that incorporates a vague time delay into fuzzy if-then rules and define a time operator that represents the relationship between an event and its fuzzy time interval. Later Maeda and Nobsada (1998) build on their earlier work and derive fuzzy rules based on actual data and propose the 'Multi-fold Multi-stage Approximate Reasoning' (MMAR) approach to predict population growth for Japan until year 2025.

Ortega, Sallum, and Massad (2000) propose the combination of fuzzy logic and non-linear dynamical systems, in order to treat some of the uncertainties and imprecision present in epidemic problems including vagueness in risk factors, hazards, the force of infection, contact patterns or infected status. They propose the application of different fuzzy inference models, without providing a detailed description of how to implement the calculations in system dynamics modeling. Given that it is not clear how membership functions were defined for specific fuzzy variables and the details about the behavior of critical variables over time were not provided; it is difficult to assess how well fuzzy modeling has been incorporated in a dynamical context in this paper.

Polat and Bozdağ (2002) compare and contrast fuzzy and classical crisp rules by running a system dynamics simulation for a simple heating model that is controlled by a human operator. The authors define fuzzy rules that describe the relationship between perceptions about temperature and the desired speed of the motor of the heating machine. However, they do not consider the combination of different fuzzy variables in their analysis.

In a more recent paper, Chang, Pai, Lin, and Wu (2006) present an application of fuzzy arithmetic representations in a system dynamics context and examine the results for a customer-producer-employment model. However the fuzzy variables considered do not interact with each other in their model and the combined effect of the fuzzy variables is not studied by the authors.

Using a different approach, Campuzano, Mula, and Peidro (2010) have demonstrated that applying possibility theory and using fuzzy numbers to estimate demand and orders in a supply chain system dynamics model can be very useful, under conditions of demand uncertainty. They conclude that despite the increased complexity of their formulation, the results are improved with respect to the bullwhip effect and the fluctuations in the inventory.

In a paper that is similar to ours in spirit, Kunsch and Springael (2008) provide a system-dynamics model of carbon tax design on the residential sector using fuzzy rules. Their objective is to show how to aggregate external data driving the model. The authors neither provide complete details about how they implement their approach, nor describe the details of the behavior of fuzzy parameters during the simulation of the model.

Overall from the literature review in this area, we find that there are a limited number of studies that address the issue of combining two or more fuzzy variables in a system dynamics modeling framework. Furthermore, these papers do not explicitly provide the implementation details associated with their respective approaches. To the best of our knowledge, there is no study that addresses the implications of considering alternative fuzzification and defuzzification methods in this context.

3. The Model

The model is based on the work by Liu, et al. (2010), where an alternative version of the model was used to introduce the idea of how to incorporate multiple linguistic variables in system dynamics modeling. The model focuses on the introduction of a new product into the market where potential customers become aware of the new product and then, based on word-of-mouth information and their perception of the product's attractiveness are converted to customers. Since the model is too complex to be described in full, each component will be described separately and the interested reader can find the full model in the Appendix A.

The molecule 'Product Diffusion' developed in VENSIM (Hines, 2004) is included to represent the dynamics associated with word-of-mouth when generating new customers and the growth of the market share (Figure 1). The basic idea is that customers have contacts with others as a function of their average sociability (i.e., how many other people one meets on average). Based on the concentration of the potential customers in the whole population, a fraction of these contacts are with potential customers. Then based on the probability that a contact will generate a new customer, these contacts will convert non-customers to customers, which is defined as the 'Word-of-Mouth Conversions'.

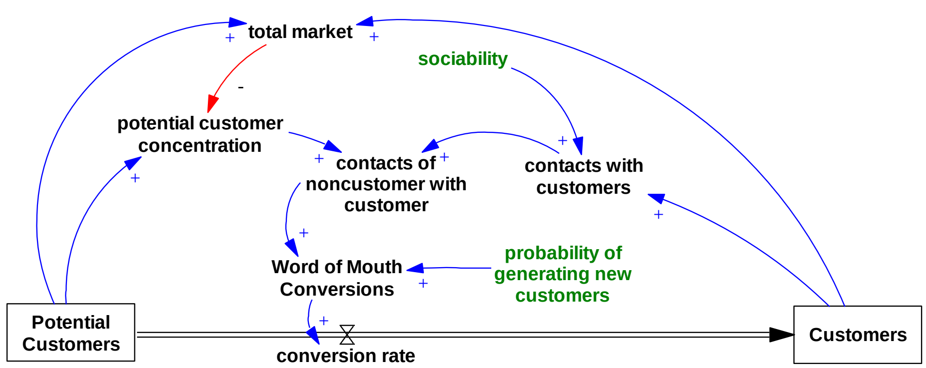

Figure 1-Product Diffusion based on Word of Mouth and Product Attractiveness

In the system dynamics model, links which are shown with a positive polarity and blue color mean that if a variable representing a cause increases, then the variable representing the effect will also increase all else being equal. For example, since potential customer concentration is the ratio of potential customers over the total market, then the causal link from 'potential customers' to 'positive customer concentration' is positive. However the link from the 'total market' to 'potential customer concentration' is negative and is indicated with minus polarity and red color meaning that higher 'total market' leads to less 'potential customer concentration' all else being equal. Furthermore, the level or stock variables are represented by rectangles and the rate by which these variables is changed is depicted with an inverted triangle.

The conversion rate from 'Potential Customers' to 'Customers' is affected by both 'Word-of-Mouth Conversions' and 'Product Attractiveness'. The latter is typically affected by several factors. In order to keep our model simple, we only consider two factors, including customer service and delivery timeliness. Delivery timeliness is dependent upon the inventory and backlog level of the firm. This section is modeled by using the 'Backlog Shipping Protected by Flow' molecule developed in VENSIM (Hines, 2004) (See Figure 2).

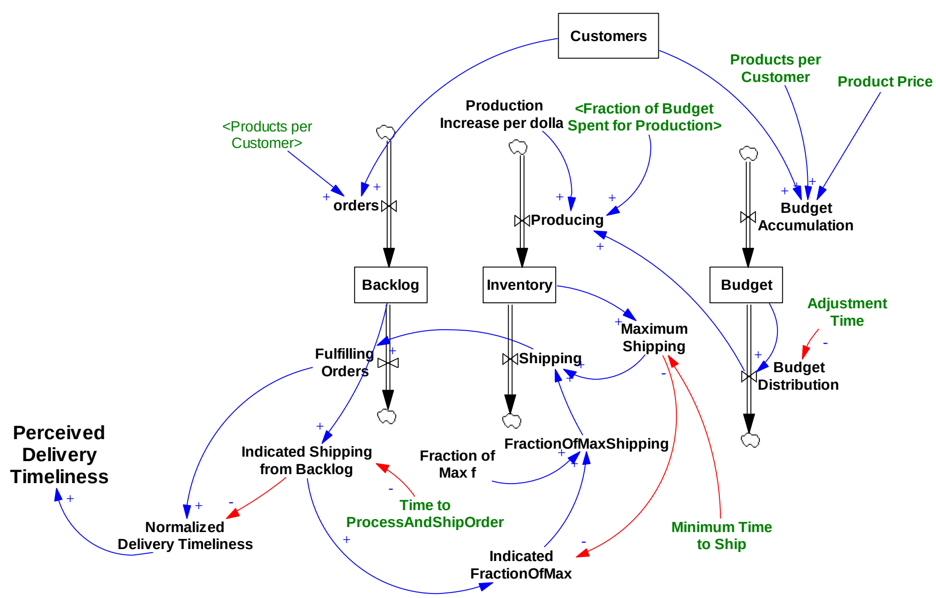

Figure 2-Backlog Shipping Protected by Flow

Delivery Timeliness which is determined by the 'Normalized Delivery Timeliness' variable is calculated as the ratio of 'Fulfilling Orders' over 'Indicated Shipping from Backlog'. The former is the actual delivery rate of orders and the latter is the desired delivery rate based on the time delay in processing and shipping orders. As described by Hines (2004), "on average orders will not exactly match what remains in stock, and hence actual shipments fall below desired shipments of orders" (p. 102). So the actual delivery rate is always less than or equal to the desired rate. Therefore, the structure of the model limits the desired delivery rate to less than or equal to the maximum possible shipping rate. Finally the 'Normalized Delivery Timeliness' is the basis for estimating 'Perceived Delivery Timeliness' that in turn affects the attractiveness of the product.

The remainder of the firm's budget is used for hiring extra sales personnel to provide the required customer service. The number of workers is changed to reach the desired number of sales personnel for the total customers, so that on average each salesperson is serving the 'Desired Sales Personnel per Customer'[2]. If the actual number of workers is less than the desired value, then more workers are hired by spending the budget assigned for this reason (Figure 3).

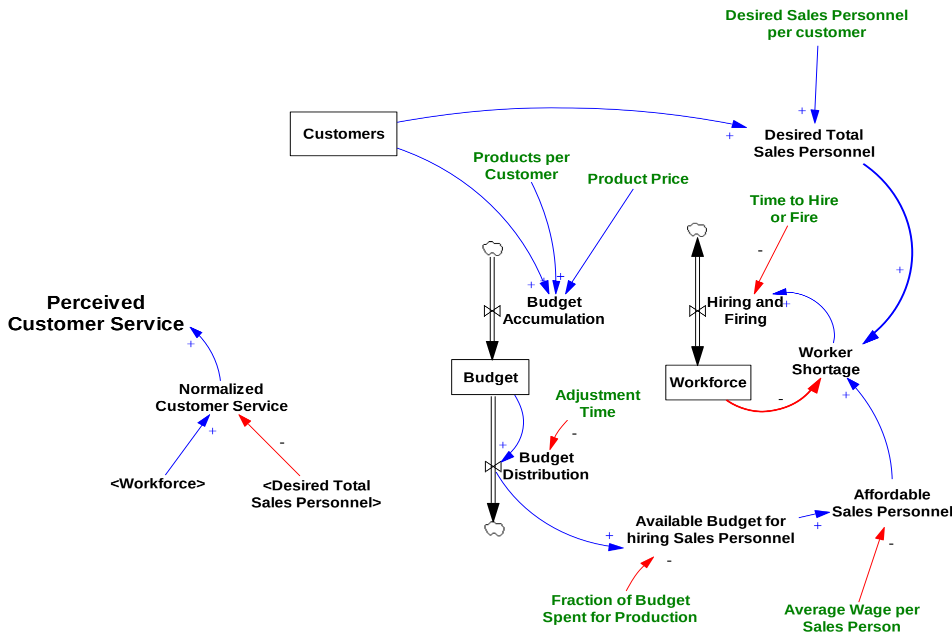

Figure 3- Workforce Change

The ratio of the number of salespeople hired (i.e. 'Workforce'), over the number of the desired workforce (i.e. 'Desired Total Salespeople') will define 'Normalized Customer Service', a normalized value between zero and one, which describes the customer service condition for the product. Consequently, the customers' perception about customer service (i.e. 'Perceived Customer Service') can be determined by the normalized customer service value. In conclusion, 'Perceived Customer Service' and 'Perceived Delivery Timeliness', together determine the variable 'Product Attractiveness'.

[2] This number is chosen arbitrarily and can be changed without qualitatively affecting the results.

4. The Fuzzification Process

As described in the introduction section, the perception variables in our model are linguistic variables which are defined by Zadeh (1975) as "*variables whose values are not numbers but words or sentences in a natural or artificial language*" (p.201). These variables are evaluated based on fuzzy logic and for this purpose, fuzzy membership functions have been incorporated to capture the vagueness inherent in the linguistic variables 'Perceived Delivery Timeliness' and 'Perceived Customer Service'.

A certain number of rules are chosen that represent different combinations of the two linguistic variables. For the sake of illustration, we use the set of rules shown in Table 1, though, others can also be used. Since each fuzzified variable has the same number of characteristics (Low, Medium and High), nine rules need to be evaluated in order to find "Product Attractiveness" (See Table 1).

Table 1 - The Nine Rules

	Perceived Customer Service	Perceived Delivery Timeliness	Product Attractiveness
1	Low	Low	Low
2	Low	Medium	Low
3	Low	High	Medium
4	Medium	Low	Medium
5	Medium	Medium	Medium
6	Medium	High	High
7	High	Low	Medium
8	High	Medium	High
9	High	High	High

The Fuzzy Rule-Based Inference System is applied to infer conclusions that consists of all the steps required to measure the adaptability of the premise of a defined set of fuzzy rules based on a given input, infer the conclusion of each rule and then to aggregate the individual conclusions to obtain the overall conclusion (Tanaka, 1997). One of the most common inference methods used is the Mamadani's method (Mamdani, 1977) because of its simple structure of min-max operations which is also used for our application and is described extensively in Appendix B.

In summary, for our model in order to find the value of each rule, based on Mamdani's Max-Min inference method, the minimum of the two perception values for that membership range (i.e. Low, Medium or High), is calculated. Then in order to find the union of the rules, the maximum value of all rules that result into a low, medium and high membership domain is found separately. As a result, in this approach, in order to evaluate the union, the maximum between rules 1 and 2 is found which is the result of representing the low membership function, the maximum for rules 3, 4, 5 and 7 is the result of representing the medium membership function and for the high membership function the maximum of rules 6, 8 and 9 is found.

5. Defuzzification Process

In order to find a crisp value for the combined effect of the two perception variables that constitute 'Product Attractiveness', defuzzification algorithms need to be applied. In our approach, two different defuzzification methods are applied in the model, i.e., the 'Largest of the Maximum (LOM)' and the 'Center of Area (COA)[3]' (See Appendix B.6). The process used to calculate the final value and the results obtained are described extensively in the following sections.

5.1 Largest Of Maximum Defuzzification (LOM) Method

In order to model the LOM defuzzification method, at each time step of the simulation, the maximum membership value among all rules is found by the 'max value' variable (See Appendix A.2). Whether the 'max value' corresponds to a *low*, *medium* or *high* characteristic, the corresponding function value is used to defuzzify the μ_x value for the variable 'Product Attractiveness based on the LOM (i.e. x). If it corresponds to the low membership function, then the defuzzified value is found by the equation $x = (1 - \mu_x)/2$. Also, for the medium membership function, among the two sides which have different formulations, only the right side formulation (i.e. $x = (2 - \mu_x)/2$) is used because it corresponds to larger x values as compared to the left (i.e. $x = \mu_x/2$). In the case of the high membership function, the defuzzified value would be $x = (\mu_x + 1)/2$.

In order to analyze the effect of the fuzzy linguistic variables on the model behavior, one can analyze a number of variables. For example, after running the simulation for the LOM defuzzification method, the 'Conversion Rate' of 'Potential Customers' into 'Customers' over a time horizon of 300 weeks is shown in Figure 4 [4].

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[3] In the literature sometimes the term 'Center Of Gravity (COG)' is used, even though it is computed only for a two-dimensional area.

[4] The time unit in our model is week, and throughout the paper, time refers to week.

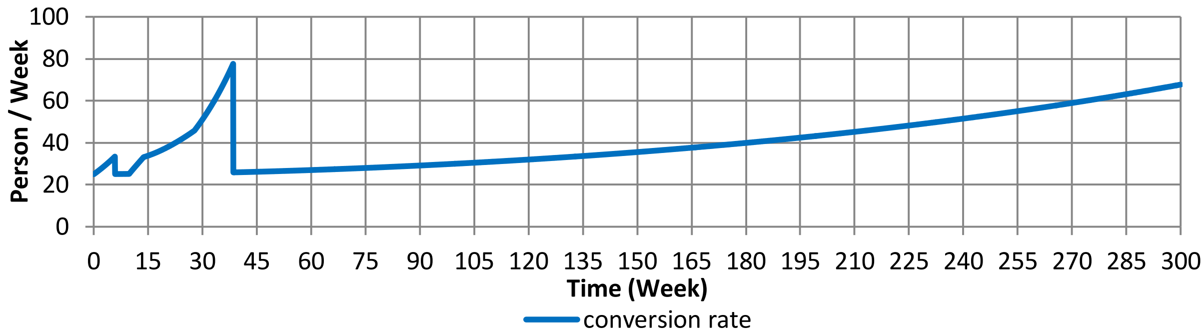

Figure 4--'Conversion Rate' Behavior in the LOM method

When we causal trace the behavior of the 'Conversion rate', we find that the main driver is 'Product Attractiveness' (in this section based on the LOM) (See Figure 5). In other words, we need to analyze the behavior of 'Product Attractiveness' to understand the behavior of the 'Conversion rate'[5]. Hence we focus on how 'Product Attractiveness' changes during the simulation, because it directly affects the conversion rate and changes of 'Potential Customers' into 'Customers'. In other words the effect of applying the fuzzy logic approach permeates the rest of the model through the 'Product Attractiveness' variable.

Even though at first glance, the behavior of the defuzzified value (i.e. Product Attractiveness) may seem reasonable, there are counter-intuitive results at certain time intervals including the sudden decreases at time points 5.8 and 38.45 and the increasing trend in time intervals 9.7 to 13.75 and also 27.75 to 38.45 (shown in the red circle in Figure 5). During these time intervals, we observe increasing defuzzified values of 'Product Attractiveness' as marked by the red circle in Figure 5 and enlarged in Figure 6.

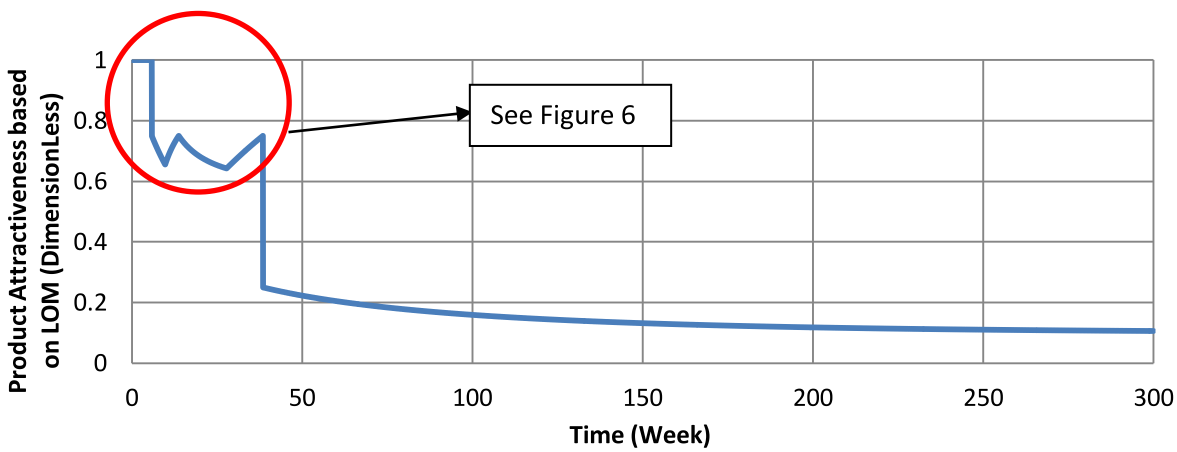

Figure 5- Defuzzified Effect of the Perceived Delivery Timeliness and Perceived Customer Service on the Product Attractiveness based on the LOM Defuzzification Method

[5] We thank the reviewers for bringing this to our attention.

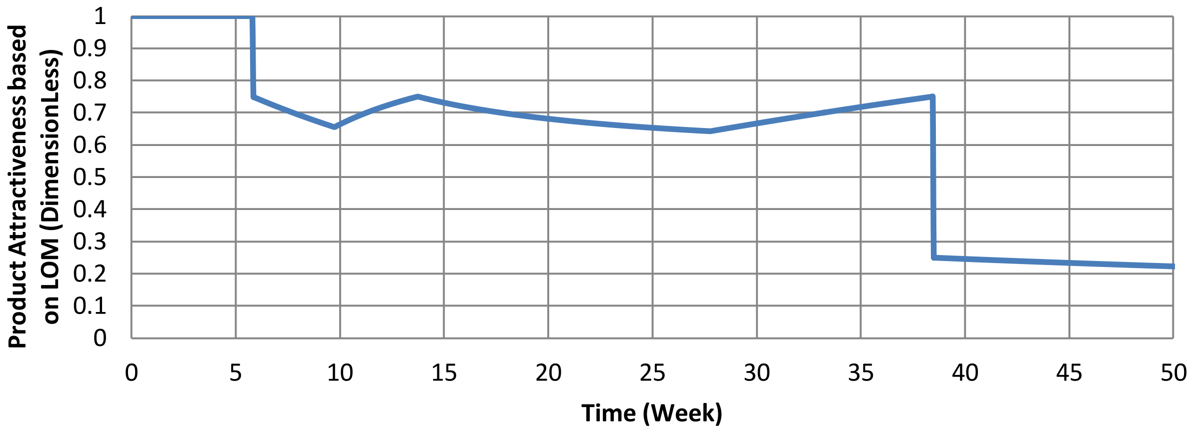

Figure 6- Product Attractiveness based on the LOM - Increasing Behavior at Some Time Intervals

On the other hand, during the simulation, 'Normalized Delivery Timeliness' and 'Normalized Customer Service' are decreasing continuously (See Figure 7). This suggests that the perceived product attractiveness also should be continuously decreasing. In the following, we study the underlying mechanism to understand the inconsistent increasing behavior during the time intervals 9.7 to 13.75 and 27.75 to 38.45.

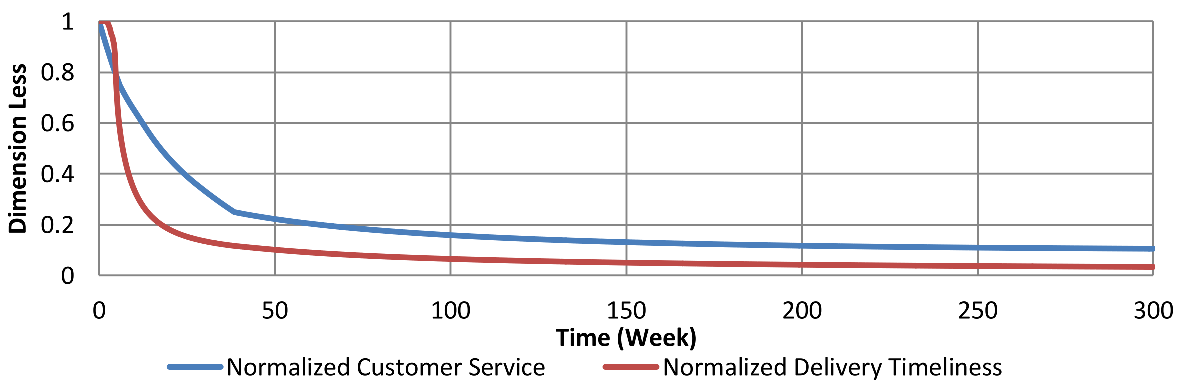

Figure 7- Normalized Delivery Timeliness and Normalized Customer Service

Initially, at the start of the simulation, 'Product Attractiveness' remains constant at 1 for some time. In this interval specifically until time 4.8, rule number 9 has the maximum output and thus influences the calculation of the value of the defuzzified variable. Rule 9, selects the minimum between 'Perceived Customer Service: *High*' and 'Perceived Delivery Timeliness: *High*'. During this time interval, the membership values associated with the antecedent 'Perceived Customer Service: *High*' are the lowest among the two, and decreases during this interval from 1 to 0.5277. This means that the calculated defuzzified values should also be decreasing from 1 to 0.76 over time, if mapped to the x axis, or graphically the calculated defuzzified values should be moving in the direction of the red arrow shown in Figure 8. However, the defuzzified values remain constant at 1 according to the LOM calculations, which assigns the largest value to the maximum membership value found. This result is not reasonable for the observed conditions described above.

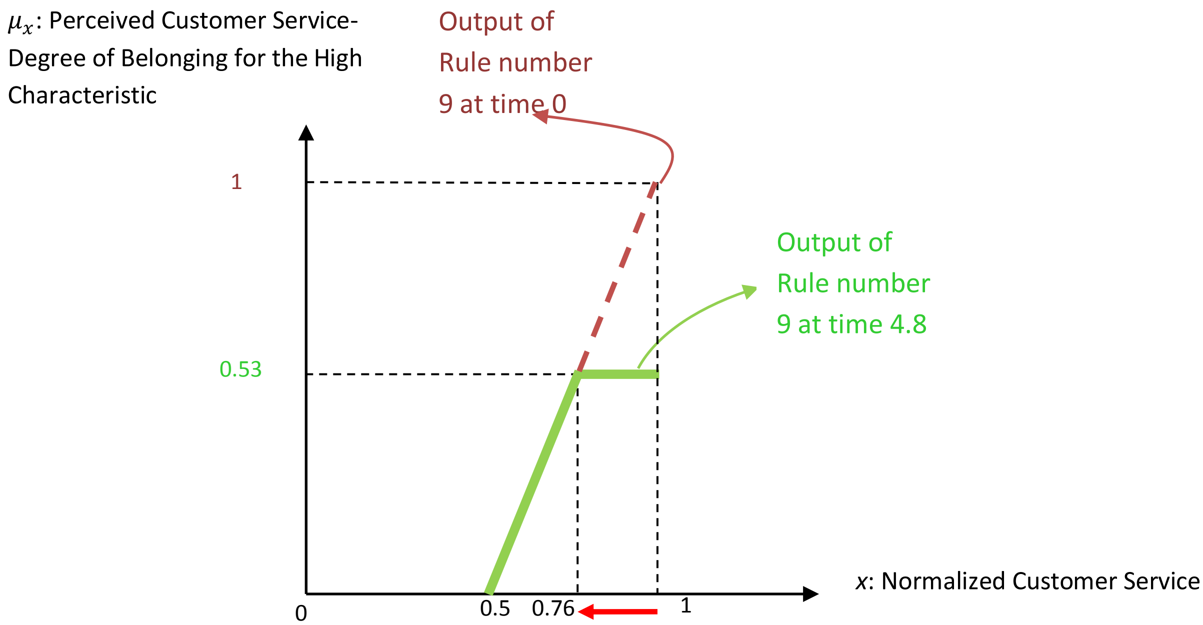

Figure 8-Impact of Rule 9 on the Defuzzified Value at the Beginning of the Simulation

Furthermore, during the time interval 9.7 to 13.75, 'Product Attractiveness' increases from 0.6544 to 0.7499 where Rule 5 has the maximum value and therefore influences the defuzzified values representing product attractiveness. Rule number 5 uses the medium membership values of both linguistic variables, Perceived Customer Service and Perceived Delivery Timeliness, to generate the 'medium' membership function output.

We observe that from time step 9.7, 'Perceived Delivery Timeliness: *medium*' has the minimum membership value (μ_x) when considering the values of the two linguistic variables. At time step 9.7 and onwards, the membership value (μ_x) of 'Perceived Delivery Timeliness *medium*' decreases from 0.6929 to 0.4998, while simultaneously the membership values for 'Perceived Delivery Timeliness *low*' increases from 0.3070 to 0.5001 (See Figure 9). In other words, the orders are delivered with higher delay than before, and the decrease of the membership value for medium should be considered with the changes of the membership values for the other characteristics collectively, to realize the actual condition of delivery timeliness.

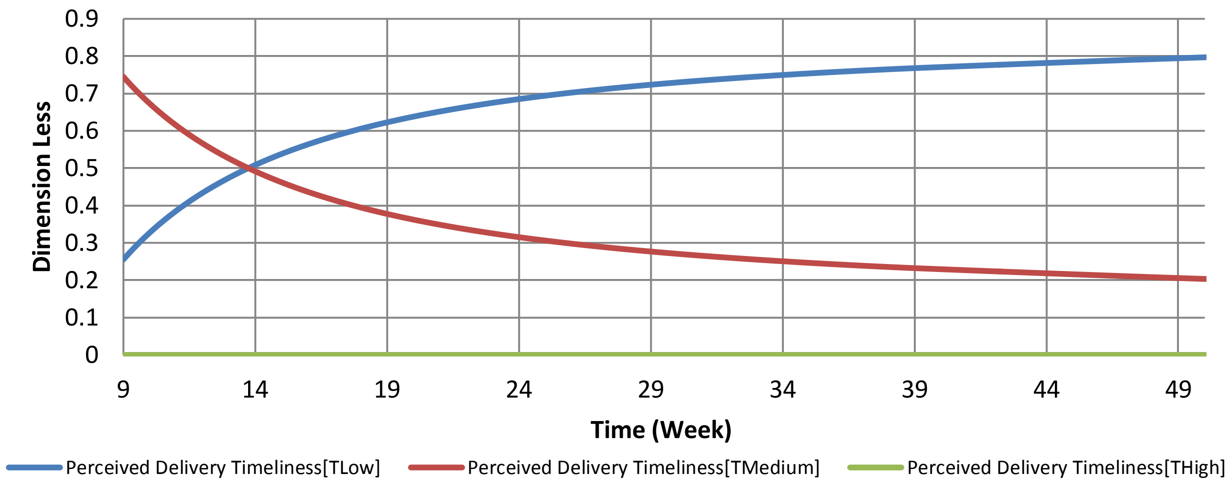

Figure 9- Perceived Delivery Timeliness in the Time Interval 9 to 50[6]

However, this behavior is not captured by the LOM defuzzification method and that is one of the disadvantages of the LOM approach. While the membership value (μ_x) of 'Perceived Delivery Timeliness*: medium*' decreases, LOM provides higher values of the defuzzifying effects on product attractiveness. In other words, the LOM defuzzified values are moving along the red arrow over time, whereas in this time period, 9.7 to 13.75, the LOM defuzzified value should be moving along the left blue arrow (See Figure 10). The dashed red arrow shows the movement of the value of the defuzzified variable at the time period 9.7 to 13.75, whereas the more reasonable movement should have been along dashed blue arrow.

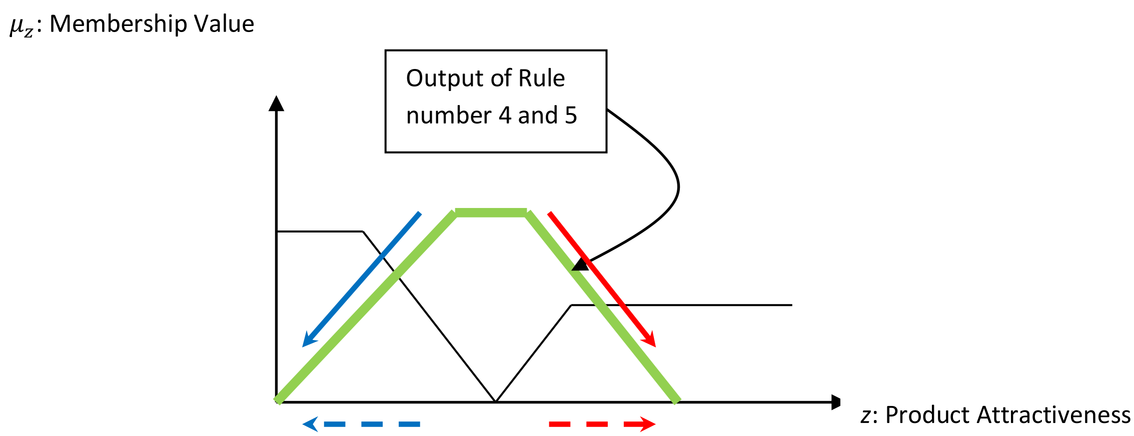

Figure 10- The Change of LOM Values Over Time

The same exact situation occurs during time interval 27.75 to 38.45, when 'Product Attractiveness' increases from 0.6424 to 0.7499 (See Figure 6). At time point 27.75 and

[6] The 'Perceived Delivery Timeliness: *high*' displayed in green, coincides with the x-axis having a value of zero in this time interval.

onwards, Rule 4 still has the maximum value, but instead of its first antecedent the 'Perceived Delivery Timeliness: *low*', the other antecedent 'Perceived Customer Service: *medium*' obtains a lower membership value (μ_x), and based on the LOM calculations, influences the defuzzified values representing product attractiveness. Although, in this interval, 'Perceived Customer Service: *medium*' is decreasing from 0.7148 to 0.5, its membership values for 'Perceived Customer Service: *low*' simultaneously increases from 0.2851 to 0.4999 (See Figure 11). In other words, the customer service is less satisfactory than before. Again as described earlier, this behavior is not captured by the LOM defuzzification method (See Figure 10).

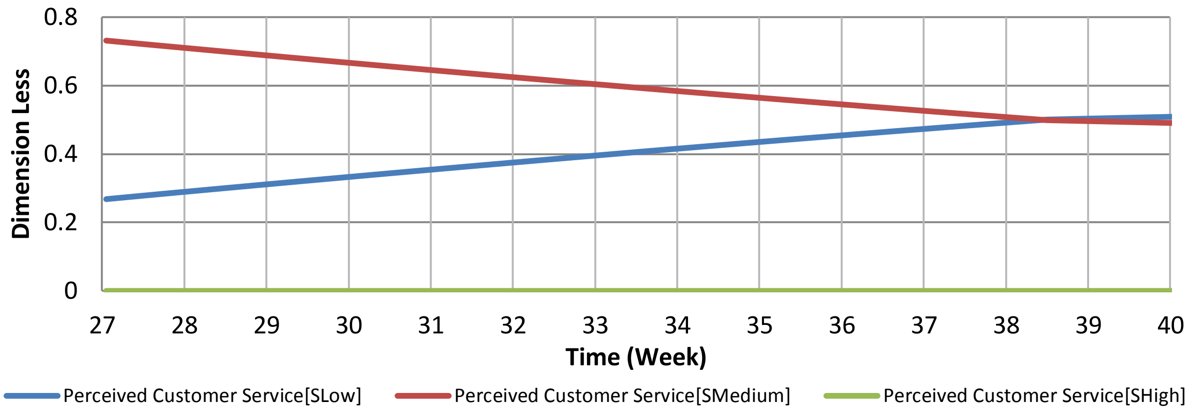

Figure 11- Perceived Customer Service in the Time Interval 27 to 40 [7]

If the defuzzified values had moved along the blue arrow, the sudden decrease of 'Product Attractiveness' from 0.7499 to 0.2495 at time point 38.45 should not have occurred. At this time step, 'Perceived Customer Service: *low*' gets a higher value (i.e. 0.5008) than 'Perceived Customer Service: *medium*' (i.e. 0.4991), and so instead of Rule 4, now Rule 1 which has the maximum value of 0.5008 among all rules, influences the defuzzified values representing product attractiveness. Rule number 1 generates 'low' membership function as its output, and due to the LOM calculation method, causes the defuzzified values to jump suddenly from point '*A*' to point '*B*' (See Figure 12).

[7] The 'Perceived Customer Service: *high*' displayed in green, coincides with the x-axis having a value of zero in this time interval.

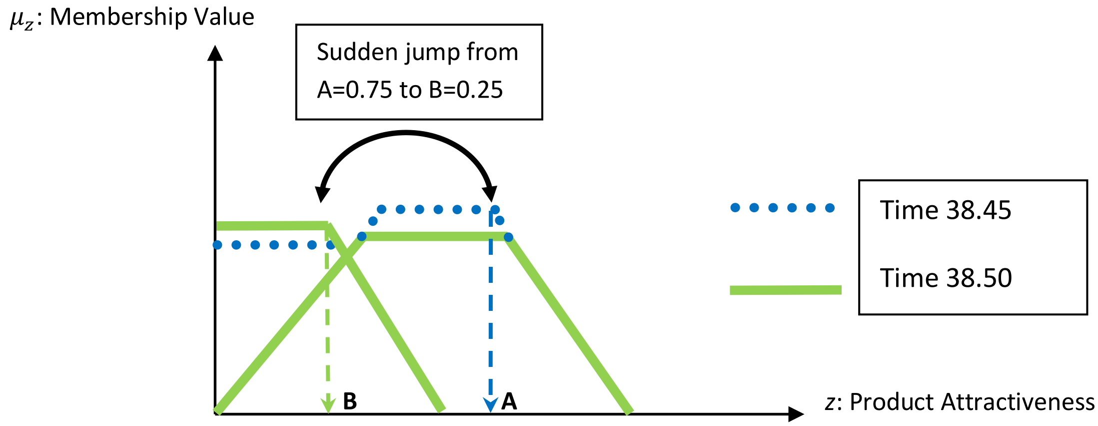

Figure 12- The Sudden Decrease at Time Point 38.45 (Week)

From this point and until the end of the simulation, Rule 1 has the maximum value among all rules. In this interval, the antecedent, 'Perceived Customer Service: *low*' has a lower membership value (μ_x) and determines the output for Rule number 1. Therefore, the resulting defuzzified values represented by 'Product Attractiveness', decrease continuously until the end of the simulation, without demonstrating any further unreasonable behavior.

5.2 Center Of Area Defuzzification (COA) Method

The Center of Area (COA) defuzzification method, calculates the weighted mean of the fuzzy area which is defined by the union of the maximum membership values for each domain value that is associated with the interface of the nine rules (See Appendix B - Figure B.4, displayed by the shaded blue area). For this purpose, and in order to incorporate the COA defuzzification method in the VENSIM model, we need to devise some approach to find the area under the boundary that is shown with the red color curve in Figure 13.

For this purpose, we find the red boundary of Figure 13, at each time step of the simulation, by obtaining the maximum membership value associated with the rules 1 and 2 representing the *low* characteristic, the maximum membership value associated with rules 3, 4, 5, and 7 representing the *medium* characteristic, and the maximum membership value associated with the rules 6, 8, and 9 representing the *high* characteristic (See Appendix B.3), that are modeled by the three variables 'max valueL', 'max valueM', and 'max valueH', respectively (see Appendix A). These variables represent the membership values for each domain value shown by the two-headed arrows in Figure 13.

Then the minimum between the values max valueL, max valueM, and max valueH and the corresponding membership values are found for the low membership function as, $\mu_x=1-2x$, for the medium membership function, left side as, $\mu_x=2x$ and right side as, $\mu_x=2-2x$, and for the high membership function as $\mu_x=2x-1$.

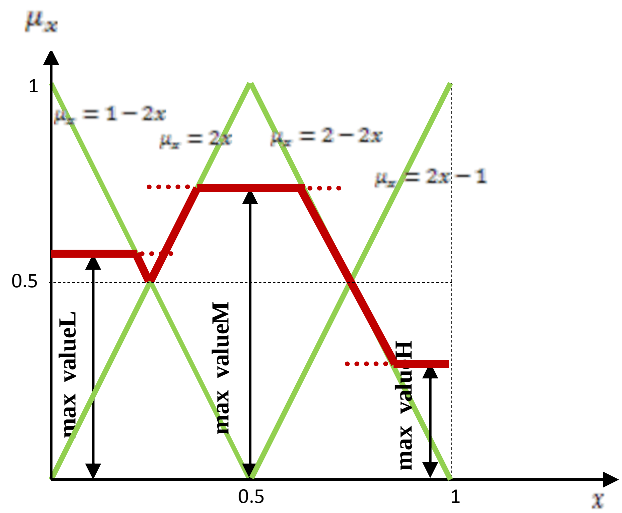

Figure 13- COA Calculation

In other words, according to Figure 13, for each membership function (corresponding to a characteristic (low, medium, high)), the value of μ_x chosen for every domain value *x* (i.e. a vector of 10000 values between 0 and 1 with a step size of 0.0001) is the minimum between the membership value associated with the membership function for that domain value and the maximum membership associated with the two-headed arrow shown in the same figure. The minimum values between these two concepts will result into the red curve boundary shown in Figure 13. Finally the value of Center of Area is calculated by using the approximation of $z_0 = \frac{\sum \mu_x x}{\sum \mu_x}$ for the integral $z_0 = \frac{\int \mu_x x dx}{\int \mu_x dx}$ at each time step (See Appendix B.6).

One would expect that the overall behavior of the defuzzified value represented by 'Product Attractiveness' to be consistent with the behavior of the two linguistic variables in the sense that when the delivery timeliness decreases and the customer service deteriorates, the COA value should also generally decrease (see Figure 14). However, counterintuitive results are observed for the interval starting at time step 4.85, for which the corresponding value of the COA is 0.5666 which then increases to 0.5755 at time step 5 as marked by the red circle in and enlarged in Figure 15.

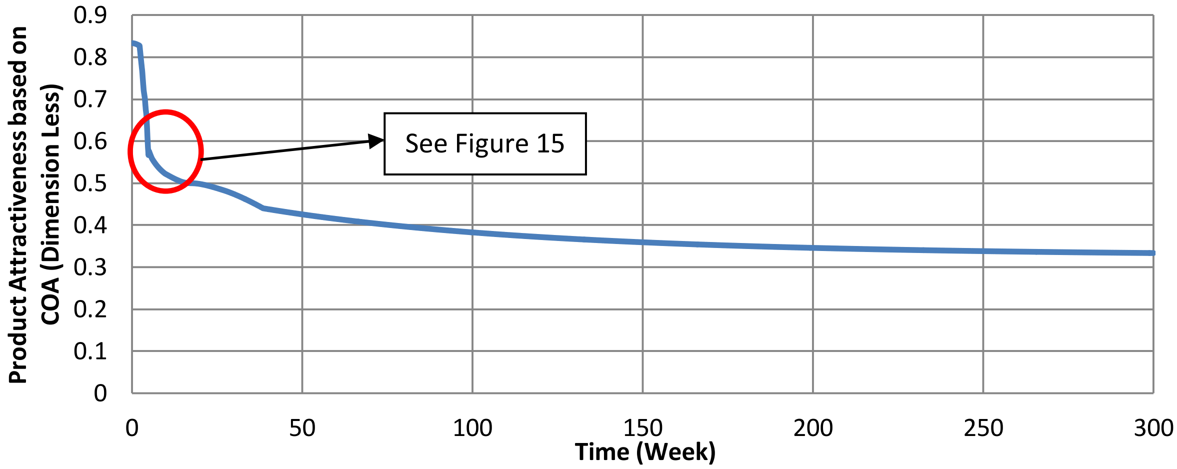

Figure 14- The Defuzzified Effect of Product Attractiveness based on the COA Defuzzification Method

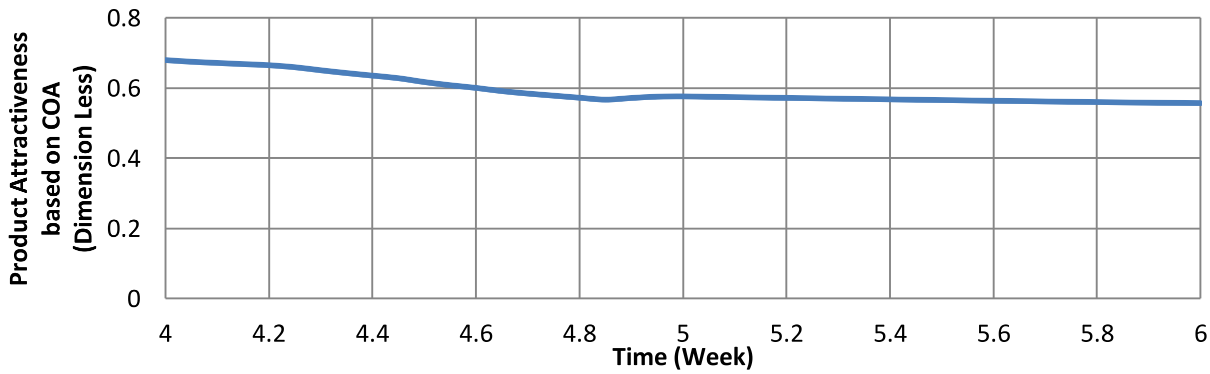

Figure 15- Counterintuitive Results based on the COA Defuzzification Method

In order to understand the underlying mechanism for this behavior, we need to study the values of max valueL, max valuM and max valuH during the time interval 4.85 to 5. The results show that the value of 'max valueL' remains zero which corresponds to the maximum value of the Rules 1 and 2 during this period. At the same time, the 'max valueM' which is the maximum value of the Rules 3, 4, 5 and 7 keeps on increasing in this time interval from the value of 0.4286 at time 4.85, to the value of 0.4403 at time 5 (See Figure 16).

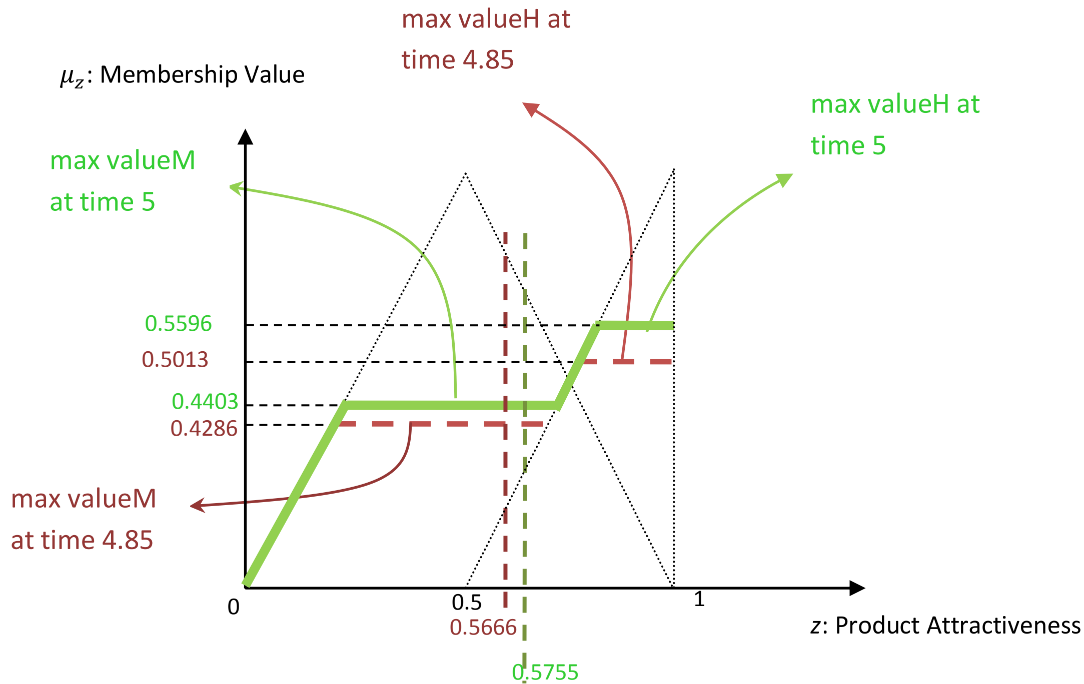

Figure 16- The resulting COA Value

However, the 'max valueH' which is the maximum value of the Rules 6, 8 and 9 decreases until time 4.85, and then starts to increase from the value of 0.5013 at time 4.85 to the value of 0.5596 at time 5 (see Figure 16). Also the values of 'max valueH' are higher than 'max valueM' (See Figure 17).

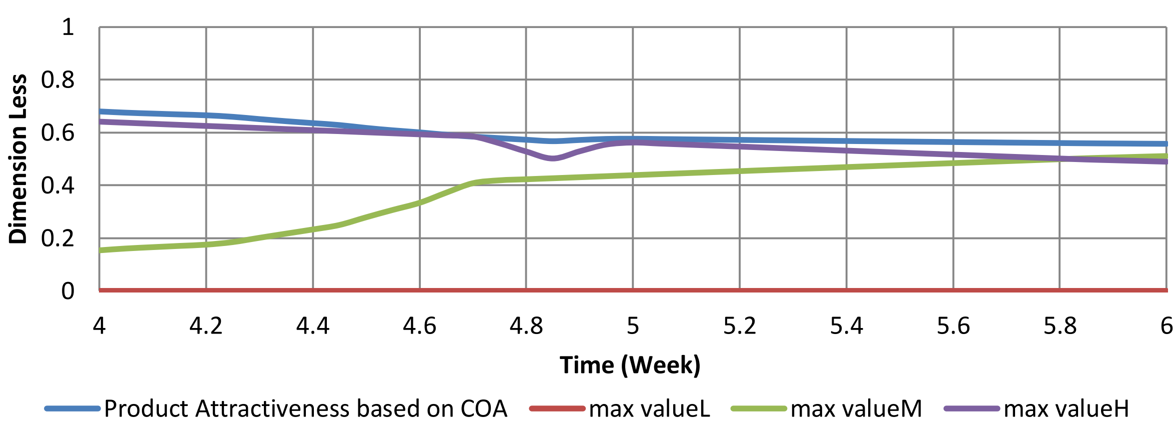

Figure 17- Counterintuitive Results based on the COA Defuzzification Method

The reason why 'max valueH' values increase after time 4.85 is due to the fact that it is determined by Rule 8 that acquires the 'high' representation of 'Perceived Customer Service' and 'medium' representation of 'Perceived Delivery Timeliness'. At this time interval, the value of 'Perceived Delivery Timeliness: *medium*' is lower than the value of 'Perceived Customer

Service: *high'* and is increasing from 0.5013 to 0.5541. So it dominates Rule 8 and consequently also causes the 'max valueH' to increase from 0.5013 to 0.5541.

Since the increase in 'max valueH' is higher than the increase of 'max valueM', the Center of Area formulation is finding a higher value for the defuzzified effect, because as the high membership value is increasing more than the medium membership value; a higher weight is put on the equivalent right half area (i.e. x>0.5666) of the graph in Figure 16. Therefore the Center of Area value moves to the right, from x=0.5666 to x=0.5755, to make the weights (i.e. the areas) on both sides equal (See Figure 16).

This analysis illustrates the challenge of combining two linguistic variables. Although the linguistic variables exhibit a declining behavior (Figure 7), the resulting defuzzified value is increasing (Figure 15) which is counter intuitive. In other words, while the medium membership values of 'Perceived Delivery Timeliness' which determines the 'max valueH', starts to increase, the high membership values of 'Perceived Delivery Timeliness' decreases, meaning that the orders are delivered later, and one would expect the product attractiveness to also decrease (See Figure 18).

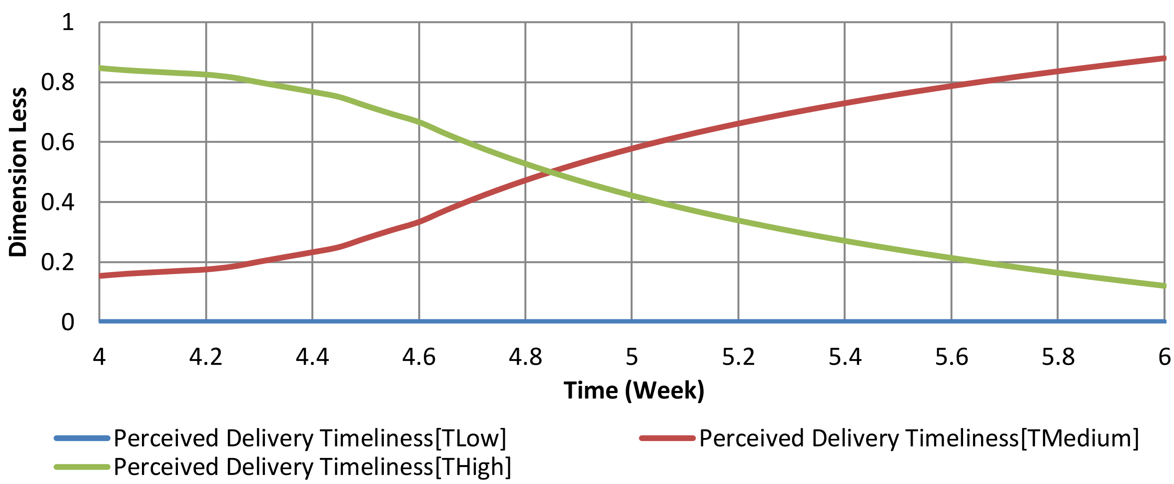

Figure 18- The Perceived Delivery Timeliness Behavior at Times 4 to 6

If during the time interval 4.85 to 5, the 'max valueM' had increased equivalently to the increase of 'max valueH', or 'max valueL' had not remained constant at zero, then the overall impact would have resulted in lower values of defuzzified values based on the COA calculation which represents product attractiveness.

This observation indicates that the counter intuitive results can be due to the inconsistent definition of the 9 rules and not the shortcoming of the defuzzification method per se. In other words the increase in the resulting value of rules which have high membership values, should be accompanied with a proportional decrease in the resulting values of the rules that have low or medium membership value and vice versa.

6. Comparison of Results

Since the results observed in the previous sections depict the effect of each defuzzification method based on combinations of the normalized values of delivery timeliness and customer service, it is reasonable to compare the two methods based on every possible combination of the two variables. We assume that we use the same set of fuzzy rules for each defuzzification approach.

For this reason we created a model that has two parameters namely the 'Normalized Delivery Timeliness' and the 'Normalized Customer Service' (See Appendix A.2). The two respective perception variables are fuzzified based on these two parameters with exactly the same triangular membership functions described in Section 4 of this paper (Also see Appendix B). Then the defuzzified effect of the two perception variables on 'Product Attractiveness' is calculated based on the two different defuzzification methods, LOM and COA.

Subsequently a multivariate sensitivity analysis in VENSIM is run using different combinations of 'Normalized Customer Service' and 'Normalized Delivery Timeliness' ranging from 0 to 1 with a step size of 0.01. The amount of the defuzzified values for COA and LOM are plotted versus the amount of each parameter that is shown in Figure 19 and Figure 20 respectively.

Obviously the value of the defuzzified variable should have the maximum value at point (Normalized Total Service Hours, Normalized Timeliness) = (1, 1). In other words when the products are delivered in the least amount of delay and Customer Service is satisfactory, the effect of Perception on 'Product Attractiveness' has the maximum value of 1 in the LOM method and 0.833367 for the COA method. Then as we move towards zero on the 'y: Normalized Delivery Timeliness' axis and simultaneously towards 0 on the 'x: Normalized Customer Service' axis, the Product Attractiveness decreases significantly to the value of 0 for the LOM and to 0.1667 for the COA method. As can be observed by the two graphs, both methods have counterintuitive increases in some regions that are more obvious in LOM than the COA method. In the COA method, the defuzzified value decreases more continuously and smoothly, but still shows increasing behavior in some regions.

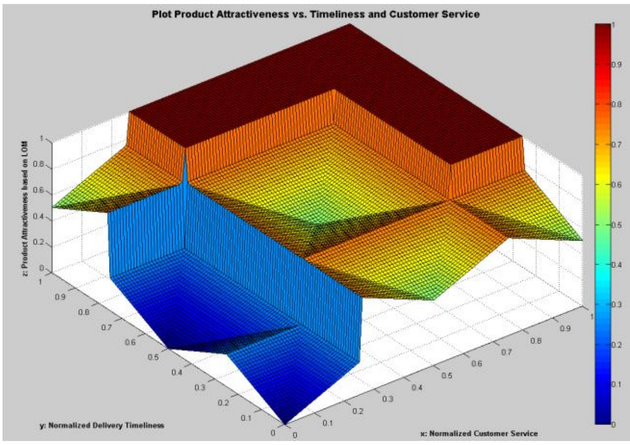

Figure 19- The LOM based Defuzzified Values vs. Normalized Delivery Timeliness and Normalized Customer Service

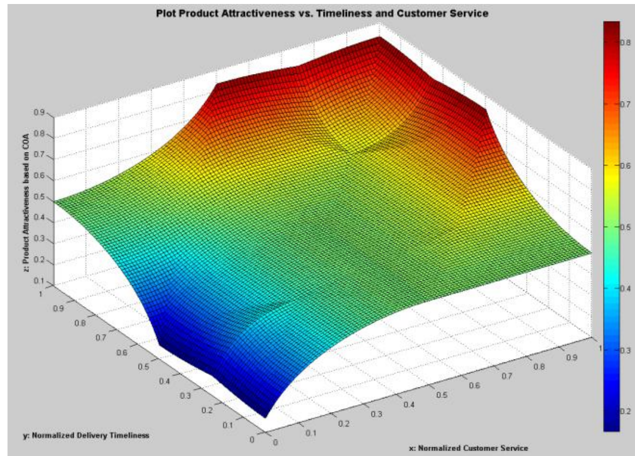

Figure 20- The COA Based Defuzzified Values vs. Normalized Delivery Timeliness and Normalized Customer Service

One of the reasons for the discontinuity and unreasonable behavior observed in the plots is due to the Mamdani Max-Min method (See Appendix B.5). Every time the minimum of the two perception variables is found, a discontinuity will result. Also whenever the maximum value between all rules is calculated, the final defuzzified value will be affected by another discontinuity. In order to verify this proposition, we propose to modify the Max-Min inference method by applying an average operator suggested in the literature, which may be seen as a heuristic. As Mizumoto (1995) suggests there are various fuzzy reasoning methods which provide better results when comparing to the Max-Min method by Mamdani (1977) that is shown by a simple fuzzy control plant model provided in his paper. Furthermore Mizumoto (1989) describes a set of averaging operators which stand in between min and max conventional fuzzy operators. The author (Mizumoto, 1989) describes that the averaging operators were already known before the emergence of fuzzy sets and illustrates the fuzzy set-theoretic points of view of different authors regarding these operators.

This modification is made in two stages as follows. In the first stage, instead of using the minimum among the membership values associated with the perceptions, the result of each rule is found by averaging the membership values associated with the two perception variables. Then at the second stage, instead of finding the maximum among rules for each domain value, the average membership value of the rules associated with each domain (i.e. low, medium and high) is calculated. Thus both modifications serve to smooth out the observed discontinuities.

We do not wish to assume that smooth behavior is "good". As we discussed in section 5, since the conditions are worsening over time (See Figure 7), so 'Product Attractiveness' should also decrease over time, and not increase at some intervals and also not change dramatically. If the model is going to be used for further analysis/prediction, and small changes in inputs lead to discrete jumps, then it would be hard for policy makers to make adjustments, or use it for policy analysis. Hence our aim is to provide insights about what leads to dramatic changes in output to guide policy making. The policy maker can choose to go for situations that will lead to smooth behavior but the goal of our model is not to prescribe this as an option, rather to illustrate what causes dramatic changes and what can be done to eliminate the discontinuities.

We execute both de-fuzzification methods after each stage. Then another set of sensitivity analyses is run in VENSIM to compare the results from implementing the modification to the initial Max-Min method. The final results are shown for the LOM and COA defuzzification methods in Figure 21 and Figure 22 respectively.

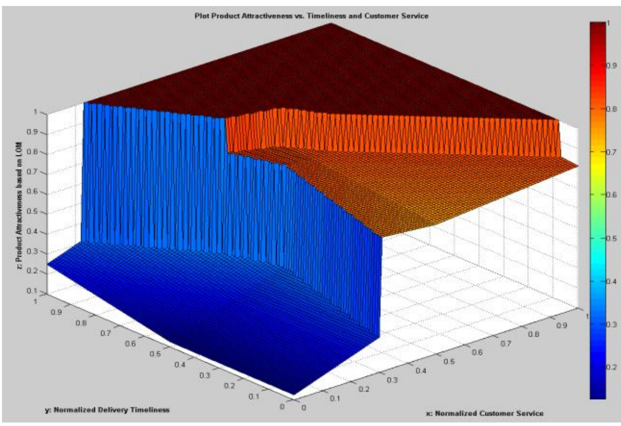

Figure 21- The LOM based Defuzzified Values vs. the Normalized Delivery Timeliness and Normalized Customer Service by Substituting the Operators with Average-Average

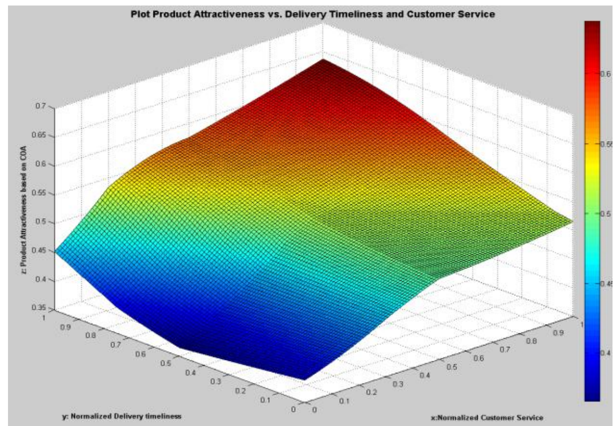

Figure 22- The COA based Defuzzified Values vs. the Normalized Delivery Timeliness and Normalized Customer Service by Substituting the Operators with Average-Average

It is apparent that by applying the average-average operations instead of the initial Max-Min operations, the final defuzzified values for both defuzzification methods have fewer discontinuities. However, still some counterintuitive results are observed by substituting the Min-Max operations. For example, in Figure 22, if 'x: Normalized Customer Service' remains constant at 0, as we move along the y-axis and the Normalized Delivery Timeliness decreases, the defuzzified values represented by product attractiveness decrease from 0.452 to about 0.365, but then counter-intuitively start to increase to 0.389. However, between the two defuzzification methods, COA presents a more continuous and smooth behavior, whereas, the LOM method exhibits a sudden increase from the value of 0.3125 to 1 as shown in Figure 21.

Overall, the suggested modifications have improved the unreasonable behavior in the original setting but have not completely resolved all the issues. The prescriptions may vary depending on the situation and may not fit for every case. Since our objective in this paper is to explore the associated challenges with incorporating the fuzzy logic in the system dynamics context, which we studied for a specific case of two linguistic variables and a certain set of membership functions, and fuzzification and defuzzification methods, it is beyond the scope of the paper to address clearly which fuzzification and defuzzification method should be preferred in and for every situation, or to perform a whole range of sensitivity analyses to answer this question.

7. Conclusion and Future Research

In this paper, fuzzy logic is applied in the system dynamics framework to enhance the ability to incorporate the vagueness associated with linguistic variables. Two different defuzzification methods, i.e., the 'Largest of Maximum (LOM)' and 'Center of Area (COA)' were applied. The LOM method is easier to compute and incorporate in a VENSIM model. On the other hand, the COA method requires the calculation of a vector consisting of hundreds up to thousands of elements due to needed precision, for every time step of the simulation. Therefore, the run time significantly increases.

Overall, the utilization of the defuzzification methods in finding crisp values for the fuzzy set in a dynamic framework leads to some counterintuitive results, but the COA method compared to LOM, is more reasonable in representing the actual real world conditions, due to the fact that it averages the membership values for the entire domain range. In general, based on our findings, by modifying the inference method from using Max-Min operations to Average-Average, the defuzzified values behave reasonably for both defuzzfication methods. Nevertheless, we still observe non-smooth changes for the COA method and also sudden changes occurring for some ranges, for the LOM method.

However, as a consequence of the defuzzification process which leads to the reduction of the representational dimensionality of the fuzzy region, a higher loss of information is concluded by the COA method due to averaging over the entire region. For instance even in the most favorable situation which is the point (Normalized Total Service Hours, Normalized Timeliness) = (1, 1), the value of COA defuzzified is 0.611; while the LOM defuzzified value is 1. In other words, the COA method behaves counter-intuitive at the boundaries of the normalized perception variables.

As a future research direction we can consider combining different fuzzy operators with alternative defuzzification methods, and also changing the number and function of fuzzy membership functions to study which fuzzy reasoning method behaves more reasonably in a system dynamics context.

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Appendix A.1- The Model

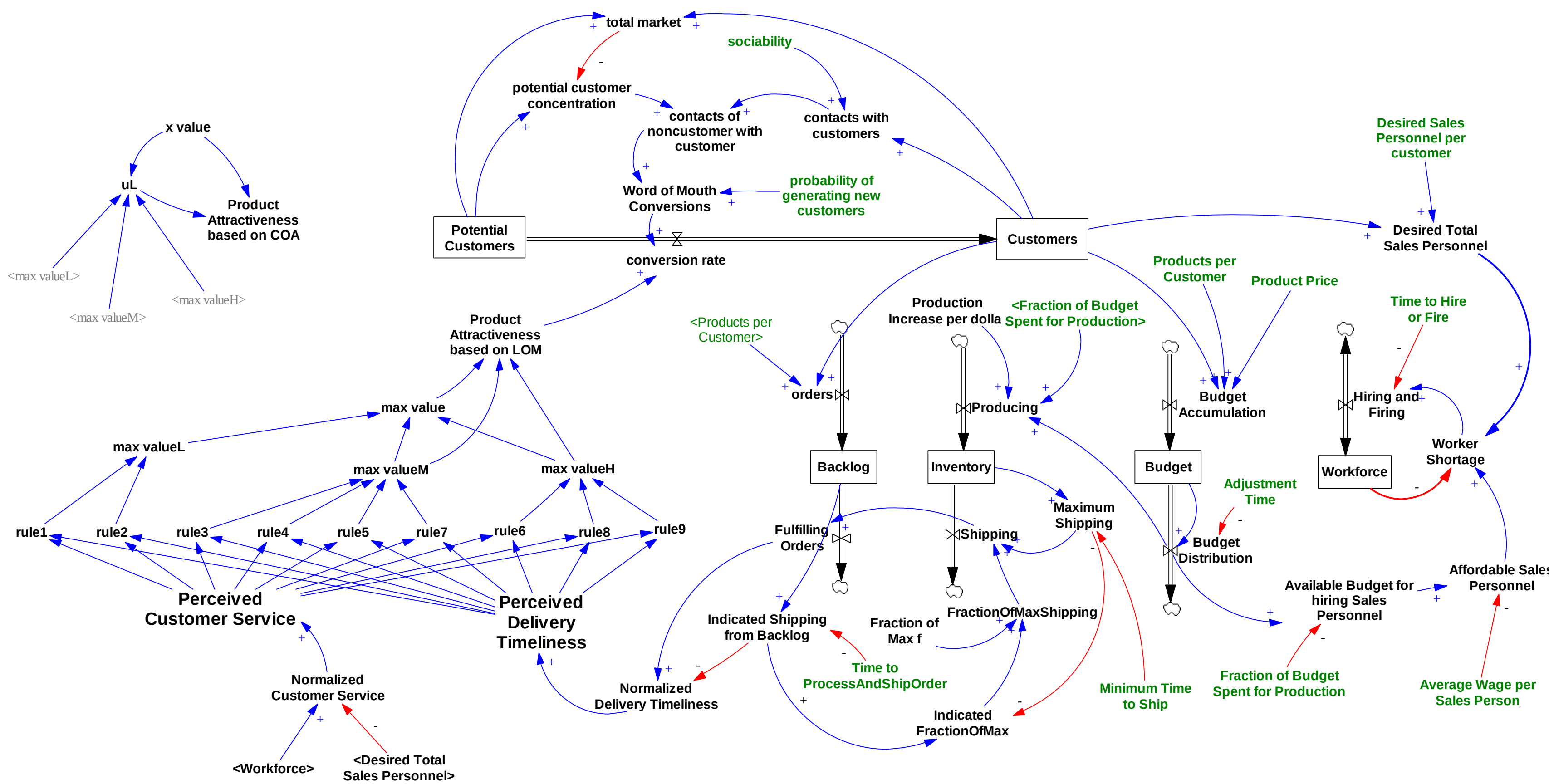

Figure A.1- The Model

Appendix A.2- The Model for Performing Sensitivity Analysis

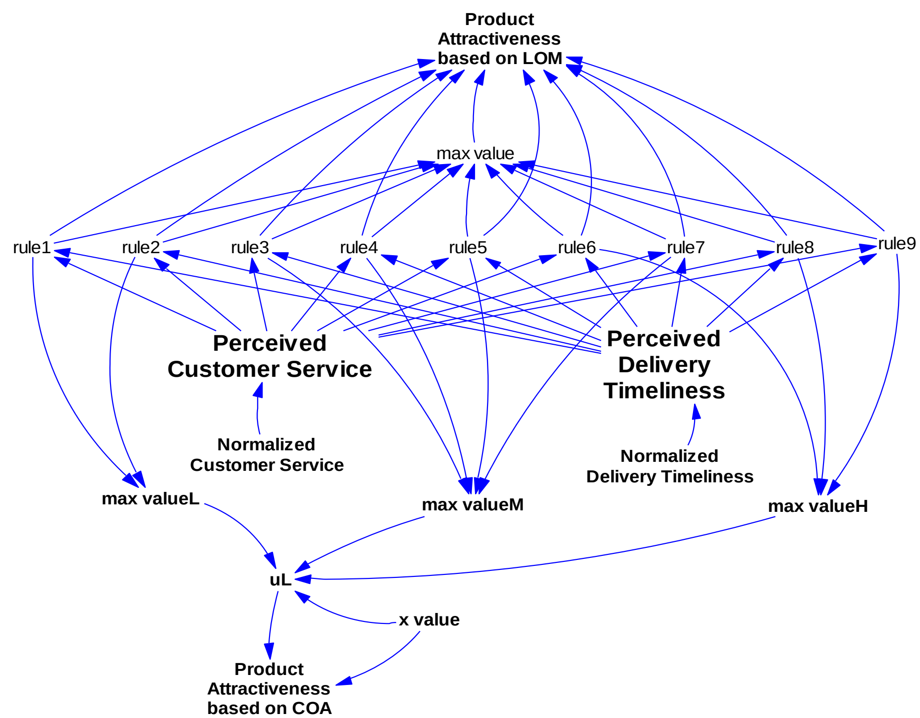

Figure A.2- The Model for Performing Sensitivity Analysis

Appendix B – Fuzzy Set Theory

B.1) Linguistic Variable:

A linguistic variable is decomposed into multiple terms represented by fuzzy sets and is described by its fuzzy space. In other words, each fuzzy set describes a semantic partition of the variable's allowable problem state. The total problem space, from smallest to largest allowable value, is called Universe of Discourse (UoD) (Cox, 1999).

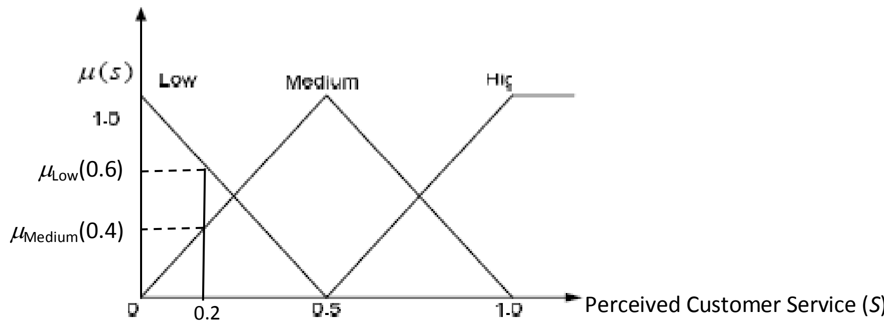

Figure B.1- Triangular Fuzzy Sets for linguistic variable

For example, in the figure above, the variable 'Perceived Customer Service' is broken down into three terms with different fuzzy sets: Low, Medium and High. In this model the UoD for 'Product Attractiveness' is 0 to 1 while the domain for the fuzzy set Low is 0 to 0.5 and is a subset of the UoD$\in$[0,1].

The fuzzy sets do not need to be symmetric but with some degree do always overlap (Cox, 1999). For instance, in the above graph, the values along the x axis demonstrate the 'Perceived Customer Service (S)' and the values along the y axis demonstrate the 'degree of membership of a fuzzy set $\mu(S)$'. A vertical line from any x value intersects with two membership functions. For example, the value 0.2 of 'Perceived Customer Service' has different degrees of Low, $\mu_{Low}(0.6)$ and Medium membership values, $\mu_{Medium}(0.4)$. Note that Figure B.1 demonstrates what is referred to in the literature as a triangular membership function.

B.2) Fuzzy Rule Based Inference System:

The fuzzy rule based inference system has four components including fuzzy rules, fuzzifier, inference engine and defuzzifier (Mendel, 1995) and the process is shown in Figure B.2. The input and output values of this system are crisp numerical values.

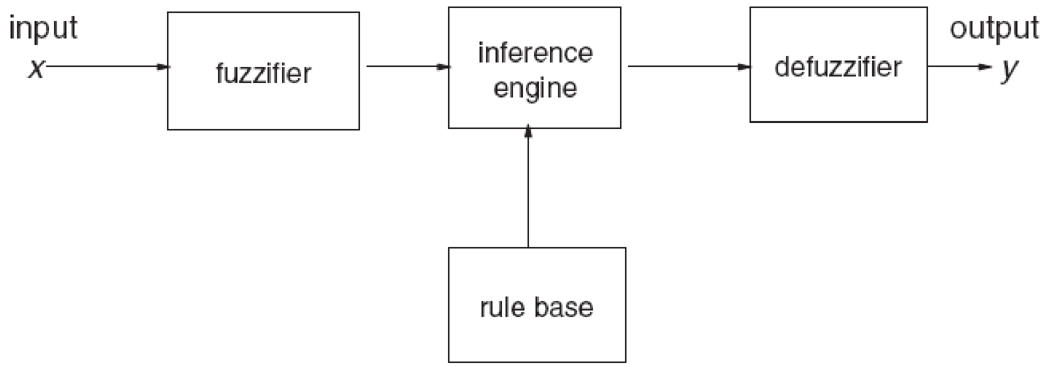

Figure B.2- Fuzzy Rule Based Inference System (Mendel, 1995)

B.3) Fuzzy Rules:

"The fuzzy rules may be provided by experts or can be extracted from numerical data" (Mendel, 1995). The rules are expressed as a collection of IF-THEN statements, e.g., "IF 'Perceived Customer Service' is Low and 'Perceived Delivery Timeliness' is Medium, THEN 'Product Attractiveness' is Low". The proposition in IF-statement is called the premise of the rule, while that in THEN-statement is called the consequence of the rule. The interested reader may refer to Mendel (1995) to learn more about the details of different methods to extract fuzzy rules.

Note that there is no a unique way to define the fuzzy rules and they could be based on expert advice or available data. In order to illustrate the effects of different types of rules, we have chosen a combination of an optimistic and pessimistic decision maker to define the rules (See Table 1).

For example, rule number two describes that if the 'Perceived Customer Service' is low (i.e. there are very few salespeople to serve the customers), and at the same time the 'Perceived Delivery Timeliness' is Medium (i.e. the orders are delivered not so late) then the product attractiveness is low. This rule is defined based on a pessimistic point of view. On the other hand, rule number 4 states that if customers perceive the customer service as medium, and the delivery timeliness as low which means orders are delivered very late, the product attractiveness is Medium. So an optimistic point of view is used to define this rule.

B.4) Fuzzification:

This stage maps crisp numbers into fuzzy sets. Our focus is the non-singleton fuzzification which the membership value is $\mu_A(u_i)$ =1 for $u_i = u'$and decreases from unity as u moves away from u'. In other words, $u'$is mapped into a fuzzy number by a fuzzy membership function. Examples of such functions are Gaussian and Triangular, which a triangular example is shown above and is applied in our research.

In the model, typical triangular fuzzy membership functions are used for the representation of individual linguistic variables which is the basis for the fuzzification process. For the sake of illustration we have assumed that the membership functions for both of the linguistic variables have three characteristics of low, medium and high as shown in Figure B.3. Depending on the need it is possible to develop a model to allow for more or fewer membership characteristics without any loss of generality.

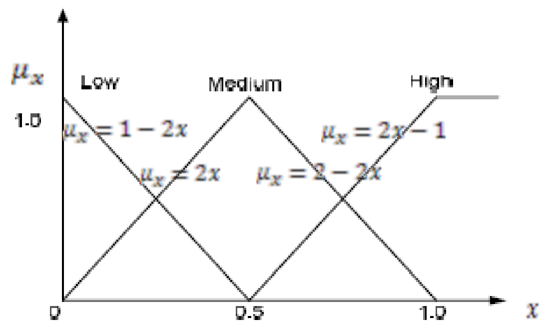

Figure B.3-The Membership Functions for the Three Characteristics Associated with Perception Variables

The membership values associated with the high, medium, and low characteristics for both perception variables (i.e. 'Perceived Delivery Timeliness' and 'Perceived Customer Service'), shown by μ_x, change as linear triangular functions of the normalized values represented by *x*, for all domains including low, medium and high (Figure B.3). The linear functions are chosen arbitrarily and the results are not sensitive to the exact membership functions chosen. In our example, if the actual shipping rate gets close enough to the desired shipping rate, then the normalized delivery timeliness (i.e. *x*) in Figure B.3 would be near 1. If for instance *x* is equal to 0.9, then the high membership function of 'Perceived Delivery Timeliness' will have the highest value (degree of truth) among all membership functions, which is 0.8, while the medium membership function would have a value of 0.2 and the low membership function would have a value equal to zero. In other words the 'Perceived Delivery Timeliness' is represented by three membership function that represent how much delivery timeliness is perceived as high, medium and low. The same concepts are applied for the 'Perceived Customer Service' as a function of the normalized customer service, which is defined by the ratio of the actual workforce to the desired workforce.

B.5) Fuzzy Inference Engine

This engine is based on Mamdani's Direct method (Mamdani, 1977) and consists of three steps as follows (Tanaka, 1997):

Step 1) Measure the adaptability of the premise of rules for a given input.

Step 2) From the adaptability obtained in the preceding, infer the conclusion of each rule.

Step 3) Aggregate the individual conclusions to obtain the overall conclusion.

In order to describe the three steps, we provide the example with three fuzzy rules in Figure B.4.

Rule 2: IF "x is Low" AND "y is Medium", THEN "z is Low."

Rule 5: IF "x is Medium" AND "y is Medium", THEN "z is Medium."

Rule 8: IF "x is Medium" AND "y is High", THEN "z is High."

In step 1, the adaptability of Rule 2 and Rule 5 is each found by selecting the minimum between the membership values of the two variables x and y.

Then in step 2, the fuzzy set in the consequence part of each rule, for example the Low fuzzy set for Rule 2, is cut by the height of the adaptability of the premise found in step 1 (i.e. Min($\mu_A(x_1), \mu_B(y_1)$).

Finally in step 3, aggregate the conclusion of all the rules by obtaining the union of all the conclusions found in step 2 which is the shaded area shown at the far right of Figure B.4.

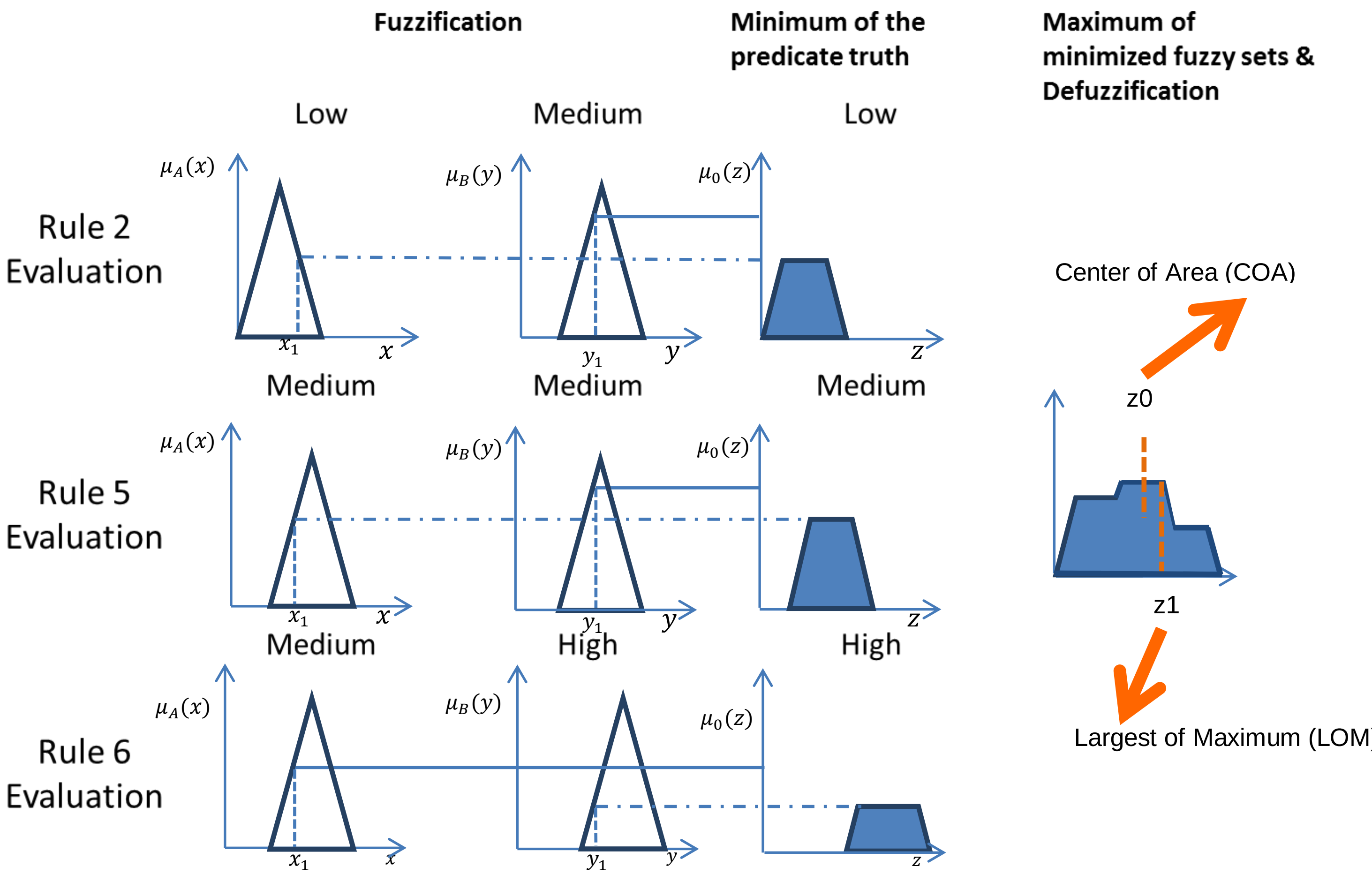

Figure B.4- Mamdani's Direct method

B.6) Defuzzification:

The final conclusion found in the previous stage is a fuzzy set. At this stage, output sets are mapped into crisp numbers. According to Cox (1999), the defuzzification has been defined as "… the process of finding the best place along the surface of the fuzzy set to drop the plumb line" (p. 306). In other words, by defuzzifying the fuzzy region, we reduce the dimension of the fuzzy region and lose some information in the sake of finding a single point to use as the inference result for our model.

A common defuzzification method used is called 'Center Of Area (COA)' of the fuzzy set which is driven by the following equation. For example, z_0 is shown in Figure B.4:

$$z_0 = \frac{\int \mu_O(z) z dz}{\int \mu_O(z) dz}$$

Another common defuzzification approach is called 'Largest of Maximum (LOM)', which selects the maximum value of membership in the fuzzy set for conclusion as follows. Also z_1 is shown in Figure B.4:

$$z_1 = \max_z \mu_O(z)$$

In the model, to find the domain with the maximum truth, the maximum value among the nine rules values and the corresponding domain, is found. For example, the maximum truth in Figure B.4 belongs to the membership function representing the *medium* characteristic. Since this point is ambiguous (i.e., it lies along a plateau), the LOM method selects the farthest edge of the plateau and drops a plumb line to resolve the conflict. As an example, in Figure B.4, in order to defuzzify the maximum value μ_{z0} which belongs to the membership function representing the *medium* characteristic, the defuzzified value z_1 is selected which is at the farthest edge and has the maximum value among all the z values belonging to this plateau value.

Appendix C – The Code

Product Attractiveness based on LOM=if then else (max valueH=max value, 1, if then else(max valueM=max value, 1-0.5*max value, 0.5-0.5*max value))
Units: Dmnl

max valueH=MAX(rule6, MAX(rule8 , rule9))
Units: Dmnl

uL[D]=MAX(MIN(max valueL, 1-2*x value[D]), MAX(MIN(max valueM, MIN(2*x value[D], 2-2*x value\
[D])) , MIN(max valueH, -1+2*x value[D])))
Units: Dmnl

max value=MAX(max valueL,MAX(max valueM, max valueH))
Units: Dmnl

Budget Accumulation=Product Price*Customers*Products per Customer
Units: dollar/Week

orders=Customers*Products per Customer
Units: gadget/Week

Affordable Sales Personnel=Available Budget for hiring Sales Personnel/Average Wage per Sales Person
Units: salesperson

Desired Sales Personnel per customer=0.2
Units: salesperson/person

Desired Total Sales Personnel=Customers*Desired Sales Personnel per customer
Units: salesperson

Producing=Fraction of Budget Spent for Production*Budget Distribution*Production Increase per dollar
Units: gadget/Week

Normalized Customer Service=XIDZ(Workforce , Desired Total Sales Personnel , 1)
Units: Dmnl

Worker Shortage=MIN((Desired Total Sales Personnel- Workforce), Affordable Sales Personnel)
Units: salesperson

Budget= INTEG (Budget Accumulation-Budget Distribution,Product Price*Customers*Products per Customer*Adjustment Time)
Units: dollar

Hiring and Firing=Worker Shortage / Time to Hire or Fire
Units: salesperson/Week

Time to Hire or Fire=2*52
Units: Week

Workforce= INTEG (Hiring and Firing, Desired Total Sales Personnel)
Units: salesperson

Normalized Delivery Timeliness=XIDZ(Fulfilling Orders , Indicated Shipping from Backlog , 1)
Units: Dmnl

Product Price=50
Units: dollar/gadget

Fraction of Max f([(0,0)-1.5,2),(0,0),(2,2)],(0,0),(0.5,0.5),(0.621176,0.604982),(0.72,0.683274),(0.818824\
,0.768683),(0.921176,0.846975),(1,0.911032),(1.11176,0.975089),(1.2,1),(1.5,1))
Units: Dmnl

Indicated FractionOfMax=XIDZ(Indicated Shipping from Backlog, Maximum Shipping , 10)
Units: Dmnl

Fulfilling Orders=Shipping
Units: gadget/Week

Indicated Shipping from Backlog=Backlog/Time to ProcessAndShipOrder
Units: gadget/Week

Maximum Shipping=Inventory/Minimum Time to Ship
Units: gadget/Week

Shipping=FractionOfMaxShipping*Maximum Shipping
Units: gadget/Week

FractionOfMaxShipping=Fraction of Max f(Indicated FractionOfMax)
Units: Dmnl

max valueL=MAX(rule1,rule2)
Units: Dmnl |

max valueM=MAX(rule3 , MAX(rule4 , MAX(rule5 , rule7)))
Units: Dmnl

Product Attractiveness based on COA=SUM(uL[D!]*x value[D!])/SUM(uL[D!])
Units: Dmnl

D:(d1-d10000)
x value[d1]= 0.0001
x value[d2]= 0.0002

x value[d3]= 0.0003
x value[d4]= 0.0004
x value[d5]= 0.0005
x value[d6]= 0.0006
x value[d7]= 0.0007
x value[d8]= 0.0008
x value[d9]= 0.0009
x value[d10]= 0.001
.
.
.
x value[d9993]=0.9993
x value[d9994]=0.9994
x value[d9995]=0.9995
x value[d9996]=0.9996
x value[d9997]=0.9997
x value[d9998]=0.9998
x value[d9999]=0.9999
x value[d10000]= 1
    Units: Dmnl

rule5=MIN(Perceived Customer Service[SMedium], Perceived Delivery Timeliness[TMedium])
    Units: Dmnl

rule6=MIN(Perceived Customer Service[SMedium], Perceived Delivery Timeliness[THigh])
    Units: Dmnl

rule8=MIN(Perceived Customer Service[SHigh], Perceived Delivery Timeliness[TMedium])
    Units: Dmnl

rule9=MIN(Perceived Customer Service[SHigh], Perceived Delivery Timeliness[THigh])
    Units: Dmnl

rule2=MIN(Perceived Customer Service[SLow], Perceived Delivery Timeliness[TMedium])
    Units: Dmnl

rule3=MIN(Perceived Customer Service[SLow], Perceived Delivery Timeliness[THigh])
    Units: Dmnl

rule4=MIN(Perceived Customer Service[SMedium], Perceived Delivery Timeliness[TLow])
    Units: Dmnl

rule7=MIN(Perceived Customer Service[SHigh], Perceived Delivery Timeliness[TLow])
    Units: Dmnl

rule1=MIN(Perceived Customer Service[SLow], Perceived Delivery Timeliness[TLow])
    Units: Dmnl

Perceived Delivery Timeliness[TLow]=if then else (Normalized Delivery Timeliness<=0, 1, if then else (Normalized Delivery Timeliness>=0:AND:Normalized Delivery Timeliness<=0.5, (0.5-Normalized Delivery Timeliness)/0.5 , 0))
Perceived Delivery Timeliness[TMedium]=if then else (Normalized Delivery Timeliness>=0 :AND: Normalized Delivery Timeliness<=0.5, Normalized Delivery Timeliness/0.5, if then else (Normalized Delivery Timeliness>=0.5 :AND:Normalized Delivery Timeliness<=1, (1-Normalized Delivery Timeliness)/0.5 , 0))
Perceived Delivery Timeliness[THigh]=if then else (Normalized Delivery Timeliness>=0.5:AND:Normalized Delivery Timeliness<=1, (Normalized Delivery Timeliness-0.5)/0.5, if then else (Normalized Delivery Timeliness>=1, 1, 0))
Units: Dmnl

timelineness perception:TLow, TMedium, THigh
Units: Dmnl

Perceived Customer Service[SLow]=if then else (Normalized Customer Service<=0, 1, if then else (Normalized Customer Service>=0:AND: Normalized Customer Service<=0.5, (0.5-Normalized Customer Service)/0.5, 0))
Perceived Customer Service[SMedium]=if then else (Normalized Customer Service>=0 :AND:Normalized Customer Service<=0.5, Normalized Customer Service/0.5, if then else (Normalized Customer Service>=0.5:AND:Normalized Customer Service<=1, (1-Normalized Customer Service)/0.5, 0))
Perceived Customer Service[SHigh]=if then else (Normalized Customer Service>=0.5:AND:Normalized Customer Service<=1, (Normalized Customer Service-0.5)/0.5, if then else (Normalized Customer Service>=1, 1, 0))
Units: Dmnl

Service hours:SLow,SMedium, SHigh

Fraction of Budget Spent for Production=0.75
Units: Dmnl

Available Budget for hiring Sales Personnel=(1-Fraction of Budget Spent for Production)*Budget Distribution
Units: dollar/Week

Potential Customers= INTEG (converting rate,1e+008)
Units: person

Production Increase per dollar=0.02
Units: gadget/dollar

Minimum Time to Ship=0.5
Units: Week

Inventory= INTEG (Producing-Shipping,Fraction of Budget Spent for Production*Budget Distribution*Production Increase per dollar*Minimum Time to Ship)
Units: gadget

Time to ProcessAndShipOrder=2
Units: Week

probability of generating new customers=0.005
Units: person/contact

contacts of noncustomer with customer=contacts with customers*potential customer concentration
Units: contact/Week

Average Wage per Sales Person=1154
Units: dollar/(salesperson*Week)

Adjustment Time=10
Units: Week

Backlog= INTEG (orders-Fulfilling Orders,orders*Minimum Time to Ship)
Units: gadget

Products per Customer=1
Units: gadget/person/Week

Budget Distribution=Budget/Adjustment Time
Units: dollar/Week

contacts with customers=Customers*sociability
Units: contact/Week

Customers= INTEG (converting rate,500)
Units: person

potential customer concentration=Potential Customers/total market
Units:Dmnl

sociability=10
Units:contact/person/Week

total market=Potential Customers+Customers
Units:person

****
.Control
***~
Simulation Control Parameters

|

converting rate=Product Attractiveness based on LOM*Word of Mouth Conversions
Units:person/Week

Word of Mouth Conversions=contacts of noncustomer with customer*probability of generating new customers
Units:person/Week

FINAL TIME = 300
Units:Week
The final time for the simulation.

INITIAL TIME = 0
Units:Week
The initial time for the simulation.

SAVEPER =
TIME STEP
Units:Week [0,?]
The frequency with which output is stored.

TIME STEP = 0.05
Units:Week [0,?]
The time step for the simulation.

Second Essay:

Simulation Modeling and Policy Analysis for Evaluating the Dynamic Impacts of a Congestion Pricing Policy for a Transportation Socioeconomic System

Abstract

This paper evaluates the impact of congestion pricing policy on mitigating traffic congestion in a cordon-based area by executing a previously formulated system dynamics framework and calibrating against the data available from the pricing scheme for the London cordon-based metropolitan area. The major considerations of this research are that individual behavior is affected by the level of congestion, the cost of driving, and the supply and demand associated with mass transit. Perceptions are captured by three separate linguistic variables and fuzzy set theory is used to evaluate the combined effects of individual perceptions on the travel mode selection and the switching behavior between travel modes. Useful insights are provided based on the simulated model which could be applied when implementing a pricing scheme policy with or without the combination with other Travel Demand Management (TDM) policies. Furthermore, the model could be used to develop a management flight simulator to assist the policy makers on deciding on critical policy variables for implementing TDM policies.

Key Words and Phrases: Travel Demand Management Policy, System Dynamics, Social Networking, Demand Dynamics, Supply Dynamics, Transportation–Socioeconomic System, Fuzzy Logic, Linguistic Variables

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1. Introduction

The objective of this paper is to provide policy insights regarding the dynamics of congestion pricing. These insights are based on a simulated version of a modeling framework developed by Liu et al. (2010) based on the system dynamics approach. The study focuses on the effects of different factors that influence traffic congestion and examines both the short-term and the long-term mitigating effects of a congestion pricing scheme in a cordon-based urban area.

Congestion pricing is a type of road pricing scheme that has been implemented in several metropolitan areas around the world including perhaps most famously the city of London. This policy is one of the 'transportation demand management (TDM)' strategies which aim to mitigate traffic congestion while still satisfying increasing travel demand without expanding road capacity (for more on TMDs see Victoria Transport Policy Institute Report (VTPI, 2010). Congestion pricing is defined by the Victoria Transport Policy Institute (VTPI, 2011) as variable road tolls that are higher under congested conditions and lower at less congested times and locations. The main purpose of the scheme is to reduce peak-period traffic volumes to optimal levels. The charging rates *can* be dynamic and change depending on the level of congestion that exists at a particular time or can vary based on a fixed schedule such as during weekday peak hours only. In general, congestion pricing can be implemented in various ways (VTPI, 2011), such as pricing a particular point in the road such as a bridge or a tunnel or a roadway section, or on a larger scale, pricing a cordon-based area similar to the pricing scheme implemented in the city of London. In London motorists are charged for driving in the central district of the city. As discussed by Liu, et al. (2010), the question that arises when implementing such a strategy is the extent that policy makers can rely on the effectiveness of the policy to mitigate traffic congestion (S. Liu, et al., 2010).

In our model, we use multiple linguistic variables to represent the perception of customers using different travel modes. It is assumed that these perceptions affect traveling behavior and the switching that occurs between travel modes. The perceptions are about the degree of traffic congestion, the opportunity cost of driving, and the travel comfort associated with metro. These perceptions are expressed in linguistic terms, (i.e., *Low*, *Medium* and *High*) and integrated into a system dynamics model to understand their dynamic behavior. The integration of multiple linguistic variables in a system dynamics framework provides an alternative way to capture behavioral variables (linguistic variables) in social system modeling. In the current model, fuzzy logic methodology that includes fuzzification and defuzzification methods has been incorporated to model multiple linguistic variables affecting traffic congestion. The model is then calibrated based on the details and data for the traffic congestion pricing policy implemented within the London metropolitan area, that are mostly available in annual reports published by Transport for London (TFL, 2011b). Accordingly, the dynamic effects of implementing a congestion pricing scheme in a cordon-based urban area are discussed. The system dynamics model is simulated to evaluate the following premises:

> *Premise 1: Revenues generated from a congestion pricing scheme can substantially improve the alternative transportation modes and the services necessary to satisfy the population's mobility needs.*
>
> *Premise 2: Improvement of alternative transportation modes can have a positive effect on the mitigation of traffic congestion in a cordon-based urban area.*
>
> *Premise 3: A congestion pricing scheme cannot effectively resolve congestion problems in short term due to the existence of material and information delays.*

In our view these premises relate to the most critical problems facing policy makers in the realm of transportation today. The exploration of these premises is discussed thoroughly in section 3 of the paper, while discussing the simulation and finding the equilibrium of the model, and also in section 5, based on the insights from the calibration of the model. Prior to that discussion, in section 2 of the paper, an overview of the model and the main reinforcing and balancing loops are presented. In section 3, the details of simulating the model, including the underlying mechanism for using different linguistic variables, the parameters of the model, and also the details and insights for finding the equilibrium of the model, are described. Later on in section 4, an overview of the data and information and sources of data is provided. Section 5 describes the specifics of calibrating the model. Further sensitivity analysis and behavioral-policy insights are provided in section 6. Finally, in section 7, we conclude with a summary of the main insights of our model.

2. Overview of the Model

We study a system dynamics model consisting of a stock and flow diagram, based on the conceptual framework developed by Liu, et al. (2010) with the modifications necessary for context. The underlying Causal Link Diagram (CLD) representation of our model which is a simplified version of the model developed by Liu, et al. (2010), is shown in Figure 23. The diagram illustrates the interactions of the various sub-systems of traffic congestion within a transportation socioeconomic system representation of a metropolitan area in terms of its main components. The current version of the model only considers two modes of travel - metro and car - and travel mode selection is configured for each mode.

A basic assumption of the model is that revenues from congestion pricing are accumulated and distributed to improve mass transit capacity. This is based on the fact that the congestion pricing scheme "also includes objectives such as investing in the Underground, improving bus services, and integrating National Rail with other transport systems" (Santos & Shaffer, 2004) (p. 178). Also Santos and Shaffer (2004) state that the Greater London Authority Act 1999 (GLA, 1999) "ensures that revenues from charging schemes will be earmarked for the mayor's transport strategy projects for at least 10 years from their implementation date" (Santos & Shaffer, 2004) (p. 178). Following this policy approach, in the model, revenue is assumed to be distributed to improve mass transit by buying extra metro cars to meet the metro demand. It is assumed that this in turn will change travelers' behaviors based on their perception of supply and demand of the public transportation mode (i.e., metro transit system).

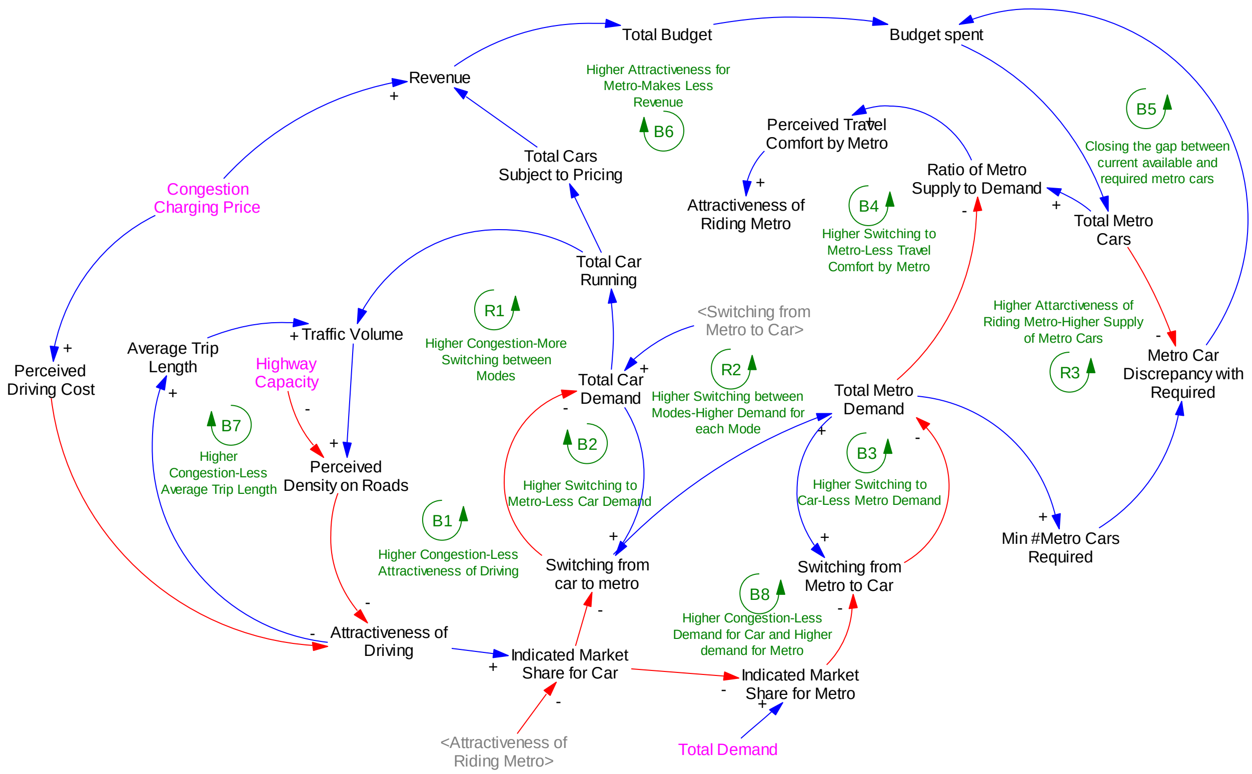

Figure 23- The Causal Link Diagram Representation

This is the focus of Loop R3 where the supply of metro cars is adjusted based on the demand for riding metro. If metro demand increases, then the supply of metro service is increased to fulfill the metro demand. Since the higher supply of metro service increases the attractiveness of riding the metro, this then increases the metro demand as more car drivers switch to using the metro. However the budget constraint associated with buying more metro cars to meet the metro demand limits the increase of metro demand (Loop B5).

The congestion pricing scheme affects the attractiveness of driving through changes in 'perceived driving cost' due to the 'congestion charging cost' imposed on drivers. When the congestion cost is imposed on car drivers, revenue is collected and is accumulated in the 'total budget' variable. However, if the attractiveness of riding metro becomes higher, and subsequently the market share for metro increases, then some of the car drivers switch to riding metro and so less revenue is collected. Loop B6 demonstrates the accumulation of revenue based on the balance between market shares of car and metro.

Similarly, congestion level on the roads, impacts the linguistic variable 'perceived density on roads'. The combined effect of 'perceived density on roads' and 'perceived driving cost' affects the 'attractiveness of driving.' Also 'perceived travel comfort by metro' is defined to capture the perception of passengers regarding riding the metro based on the supply of metro cars to its demand. If the pricing scheme is able to decrease the 'attractiveness of driving' and make drivers switch to the metro, then traffic congestion will be mitigated, which is captured by loop B2 and balanced by the increase of attractiveness of driving in loop B1. The other loops, including B3, B4, B8, R1 and R2, are complementary to loops B1 and B2 in terms of adjusting the indicated market shares of each travel mode, based on the attractiveness of each mode and switching from one mode to another. The underlying structure is described extensively later in Section 3.[8]

3. The Simulation Model

In this section, the building blocks of the simulation model are described. One of the major parts of the model concerns mode selection which is based on the attractiveness of each mode and finding the indicated market shares. In order to evaluate the attractiveness of different travel modes, recall that we use three linguistic variables that describe a user's perception with respect to the condition of these modes. These include 'perceived driving cost' for driving cost versus its value, 'perceived density on roads' for the level of traffic congestion and 'perceived travel comfort by metro' for the level of mass transit service defined in terms of its supply and demand. In order to determine the 'attractiveness of driving car (A_{Car})', the combined effect of 'perceived density on roads' and 'perceived driving cost' is evaluated. Also the 'attractiveness of riding metro (A_{Metro})' is determined based on the 'perceived travel comfort by metro'.

Individuals' perceptions are generally hard to quantify and have an inherent vagueness which makes it hard to describe them with certainty. Hence in many instances they are best represented by linguistic variables. For example, in the statement 'density on roads is perceived to be high', the premise 'density on roads' can be estimated with certainty based on the ratio of traffic volume over highway capacity. However, the attached perception level is vague and does not have a clear (crisp) value. For example, if the normalized density on roads value is 0.6, it is reasonable to infer that the perception with regard to traffic congestion is possibly not perceived as *high*, but more as a *medium* level of congestion and to some extent may even be considered a *low* congestion level, but '*high*', '*medium*' and '*low*' themselves are not well defined.

[8] The model is also indirectly related to modeling the socializing behavior of passengers. In this regard, Loop B7 demonstrates the effect of traffic congestion on the average length of travel of drivers. It could be argued that the average trip length also captures the extent to which passengers can socialize with each other. However, it requires a separate model, and we leave this aside for future research. Here we just wish to point out that any change in average trip length will assist in studying the effect of a congestion pricing scheme on the social behavior of the car passengers.

Fuzzy Set theory is one of the most popular approaches used to deal with the kind of uncertainty associated with the use of language (Zadeh, 1975). Each linguistic variable can be assumed to have three characteristics: *low*, *medium* and *high*. We assume that each linguistic variable represents an aspect of the attractiveness of each travelling mode. Typical triangular fuzzy membership functions (which define the degree of belongingness to a set) are then incorporated to capture the ambiguity inherent in the linguistic variables discussed above (see Figure 24).

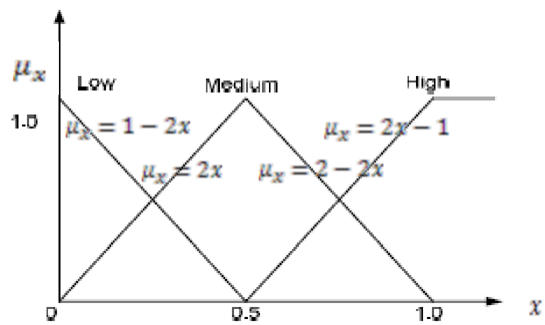

Figure 24- Membership Functions for the Linguistic Variables

In order to evaluate 'perceived density on roads', the 'normalized density on roads' is defined as the ratio of 'traffic volume' over highway capacity represented by *x* in Figure 24. The 'traffic volume' is calculated as the number of cars driving on the roads multiplied by the average value of their trip length. The 'normalized density on roads' is fuzzified into 'perceived density on roads' by the membership functions represented by Figure 24.

The 'perceived driving cost' is evaluated by capturing the effect of imposing an extra cost on drivers and how this makes driving appear less attractive for them. When the traffic congestion pricing policy is implemented, a greater burden is imposed on solo-drivers. This discourages people from driving solo and will induce them to switch to the mass transit mode. The 'congestion charging cost' is an exogenous parameter, which when divided by the 'maximum acceptable congestion charge', determines the 'ratio of the travel cost to the budget'. This ratio is normalized between zero and 1, and then fuzzified into the 'perceived driving cost' variable by using the membership functions represented by Figure 24.

Revenue is accumulated from cars that enter the charging zone. A fraction of the accumulated revenue is spent on buying extra metro cars. The ratio of number of supplied metro cars to the required number of metro cars to cover the 'total metro demand', defines the 'ratio of metro supply to demand'. This ratio is normalized between zero and 1, and then fuzzified as ‘perceived travel comfort by metro’ by using the membership functions represented by Figure 24.

In order to determine the combined effect of ‘perceived density on roads’ and ‘perceived driving cost’ that determine the ‘attractiveness of driving car (A_{Car})’, it is necessary to define individual fuzzy rules to account for the combined effect of these two linguistic variables. As linguistic variable has the same number of characteristics (*Low*, *Medium* and *High*), nine rules (defined in Table 1) need to be evaluated to find the ‘attractiveness of driving’. For the sake of illustration, the set of rules shown in Table 1 are chosen based on our intuition, though others can also be used. Note that there is no unique way to define the fuzzy rules, and they could be based on expert advice or available data.

Table 2- The Fuzzy Rules

	Perceived Density on Roads	Perceived Driving Cost	Attractiveness of Driving Car
1	Low	Low	High
2	Low	Medium	High
3	Low	High	Medium
4	Medium	Low	High
5	Medium	Medium	Medium
6	Medium	High	Low
7	High	Low	Medium
8	High	Medium	Low
9	High	High	Low

Rule 1 represents the situation where if the ‘perceived density on roads’ is *low* (i.e., there are relatively very few cars on the roads), and at the same time the ‘perceived driving cost’ is also *low* (i.e., the charging cost for entering the charging zone is low or not applied) then the ‘attractiveness of driving’ is *high*. On the other hand, rule number 9 depicts that if drivers perceive both the density on the roads and also the charging cost to be *high*, then the ‘attractiveness of driving’ is considered *low*. Other rules can be interpreted in the same manner.

In the model the ‘attractiveness of riding metro’ is solely determined by the perceived travel comfort by metro. So, the *low*, *medium* and *high* domain values of perceived travel comfort by metro define the *low*, *medium* and *high* domain value of attractiveness of riding metro respectively, and definition of the fuzzy rules is trivial in this case.

In order to find the value of each rule for driving attractiveness, Mamdani’s Max-Min inference method (Mamdani, 1977) is modified. Based on Mamdani’s Max-Min inference method, in order to find the value of each rule, the minimum of the two perception values for that membership range (i.e., *Low*, *Medium* or *High*), is calculated. Then, in order to find the union of the rules, the maximum value of all rules that result in a *low*, *medium* and *high* membership domain is found separately. As an example, the result of this inference method for rule 2 with a *low* membership consequent, rule 5 with a *medium* and rule 6 with a *high* membership consequent, is displayed by the shaded blue area in Figure 25.

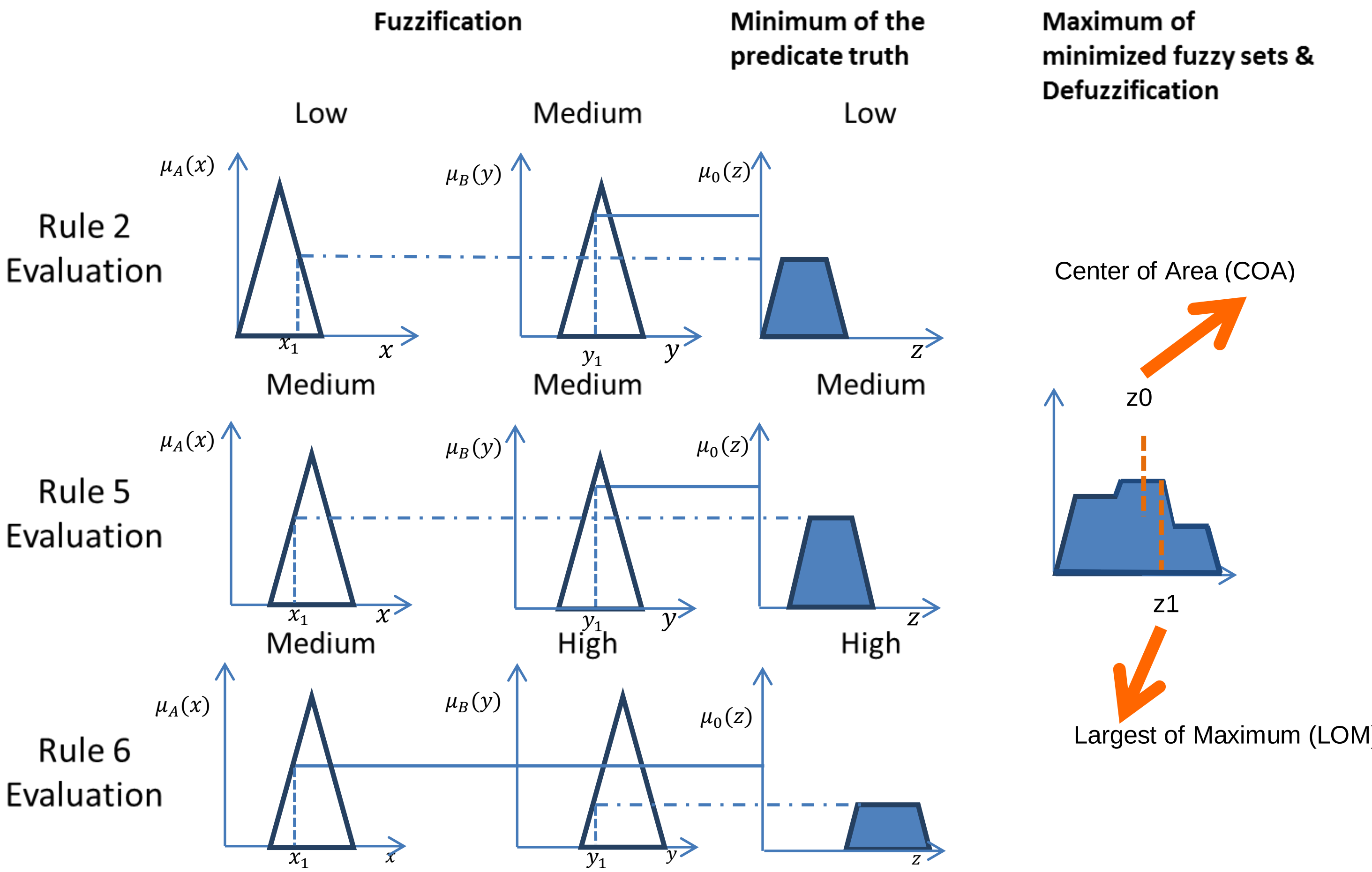

Figure 25- Mamdani's Direct method

For the model in this paper, the Max-Min method is modified to the average-average operator (Mizumoto, 1989) so that the final results are reasonable. This modified operator is discussed extensively by Sabounchi, et al. (2011). Briefly, using this method, in our model we find the value of each rule using the average of the two perception values for that membership range (i.e., *Low*, *Medium* or *High*). Then in order to find the union of the rules, the average value of all rules that result into a *low*, *medium* and *high* membership domain is found separately. As a result, in order to evaluate the union, the average between rules 6, 8 and 9 is found, which is the result for representing the *low* membership function; the average for rules 3, 5 and 7 is the result for representing the *medium* membership function; and for the *high* membership function the maximum of rules 1, 2 and 4 is found.

Finally, in order to find a crisp value for the 'attractiveness of riding metro' and 'attractiveness of driving', the Center of Area (COA) defuzzification algorithm is applied (Cox, 1999).[9] The Center of Area (COA) defuzzification method calculates the weighted mean of the fuzzy area which is defined as the union of the average membership values for each domain value that is associated with the interface of the nine rules, represented by z_0 in Figure 25. For this purpose, and in order to incorporate the COA defuzzification method in the simulation model, we need to devise an approach to find the area under the boundary of the shaded green area.

To do this, at each time step of the simulation, we find the maximum membership value associated with the rules representing the *low* characteristic, the maximum membership value associated with the rules representing the *medium* characteristic, and the maximum membership value associated with the rules representing the *high* characteristic, which are modeled by the three variables 'max valueL', 'max valueM', and 'max valueH', respectively, and hereafter are denoted by $\overline{L}$, $\overline{M}$ and $\overline{H}$ (see Figure 26).

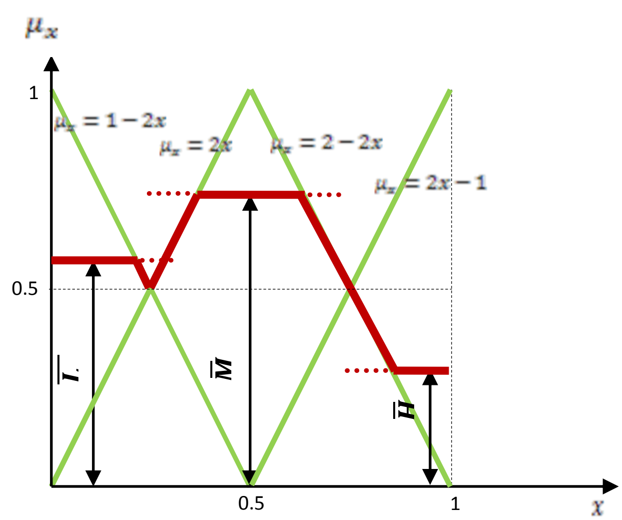

Figure 26- COA Calculation

Then the minimum between the values $\overline{L}$, $\overline{M}$ and $\overline{H}$ and the corresponding membership values are found for the *low* membership function: $\mu_x = 1 - 2x$, *Medium* membership function, left side: $\mu_x = 2x$ and right side: $\mu_x = 2 - 2x$, and *High* membership function: $\mu_x = 2x - 1$. In other words, for every x (i.e., a vector of 10000 values between 0 and 1 with a step size of 0.0001, for better approximation), the membership value chosen for x in each

[9] Research by Sabounchi et al. (2011) shows that the Center of Area (COA) defuzzification algorithm is better since the Largest of Maximum (LOM) method provides counterintuitive results at times.

domain (i.e., *low*, *medium*, *high*), is the minimum between μ_x and the maximum membership value associated with the rules for that domain, denoted by $\overline{L}$, $\overline{M}$ and $\overline{H}$. Finally the value of COA is calculated by using the approximation of $z_0 = \frac{\sum \mu_x x}{\sum \mu_x}$ for the integral $z_0 = \frac{\int \mu_x x dx}{\int \mu_x dx}$ at each time step represented by 'attractiveness of riding metro' and 'attractiveness of driving' (see Figure 27).

As Sabounchi et al. (2011) discuss, the COA defuzzification method with the average-average operator, evaluates the final defuzzified value as 0.6111 for the model in this paper, even for the most favorable situation (for example if density on roads and cost of driving are both zero). Also when normalized density on roads and cost of driving are both one, then the defuzzified value of attractiveness of driving the car is calculated as 0.3889. So it is reasonable to normalize the defuzzified values based on the COA method, between zero and one (see Figure 27).

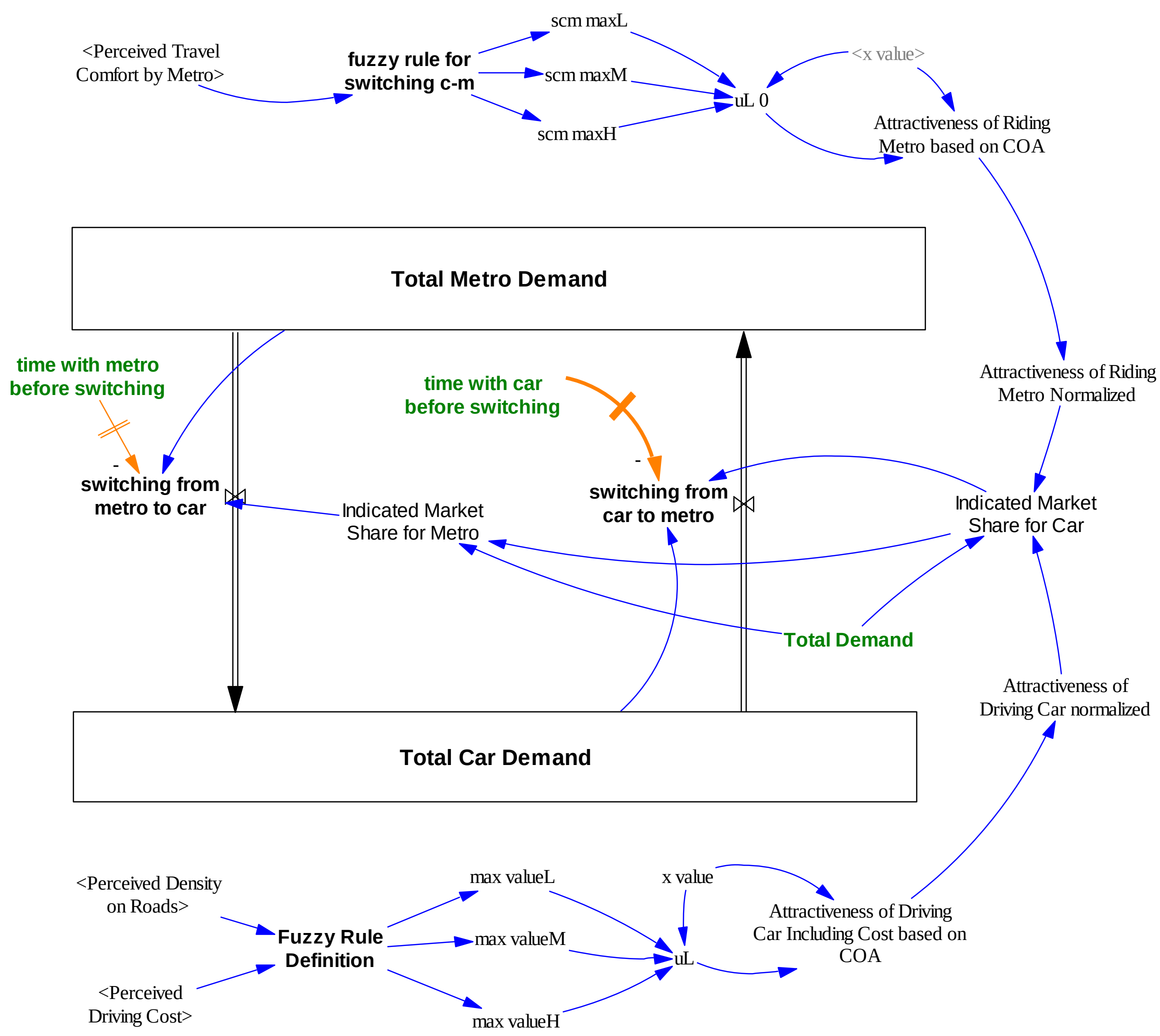

Figure 27- Mode Selection

In our model, to find the indicated market shares for car (I_{Car}) and metro (I_{Metro}), we choose to adopt Sterman's (2000) approach.[10] As Sterman (2000) states, "market share is determined by the attractiveness of each firm's product relative to the attractiveness of the other firms' products" (p. 392). The author provides a formulation for relative market share of each product. In our model, the total demand for metro and car characterizes the total demand in the model which has a constant value and does not change during the simulation period. In other words, for simplicity, the model assumes the immigration, tourists entering the zone, and employment increase rates to be zero. Similar to Sterman's (2000) approach, the indicated market share for car and metro mode is calculated as follows[11]:

$$Indicated\ Market\ Share\ for\ travel\ mode\ i = Total\ Demand\ \times \frac{Attractiveness\ of\ travel\ mode\ i}{\sum_{j=1}^{2} Attractiveness\ of\ travel\ mode\ j} \quad (1)$$

Since the total demand is equal to the sum of indicated market shares for car (I_{Car}) and metro (I_{Metro}), the indicated market shares for car and metro modes are:

$$I_{Car} = A_{Car} * (I_{Car} + I_{Metro})/(A_{Car} + A_{Metro}) \quad (2)$$

$$I_{Metro} = A_{Metro} * (I_{Car} + I_{Metro})/(A_{Car} + A_{Metro}) \quad (3)$$

Based on the attractiveness of car (A_{Car}) and metro (A_{Metro}), the above equations find different values for the initial values of metro (I_{Metro}) and car (I_{Car}) to put the model in equilibrium. As we demonstrate in Section 5, the results reasonably match the data, indicating that our approach is reasonable.

Next, based on the difference between the indicated market shares and the total travel mode demand, the switching behavior of passengers to the other mode will be determined. If the total car demand is higher than the indicated market share for car, then drivers switch to riding the metro and vice versa. Since switching takes place with a time lag, the constant 'time with car before switching' is defined in the model. Similarly, switching by metro passengers to cars assumes some time delay, which is captured by the parameter 'time with metro before switching'. The part of the model that determines the indicated market shares is shown in Figure 27. We assume that part of the revenue collected from congestion pricing is allocated for

[10] An alternative for finding the indicated market shares I_{Car} and I_{Metro}, is proposed by Ben-Akiva and Lerman (1985) which is to use the common discrete choice models popular in the transportation literature, specifically, the logit model. However, this requires us to assume that the attractiveness values A_{Car} and A_{Metro} , include a random term which is presumed to be independent and identically distributed (Dell'Orco and Kikuchi, 2004). Nevertheless, as Dell'Orco and Kikuchi (2004) argue, "from a theoretical point of view, the logit model cannot adequately deal with situations in which the variances of the attributes are different" and propose the use of possibility theory to compare the utilities of different alternatives in such situation. For further discussion see Appendix A.

[11] The interested reader can also check Sterman (2000) on the advantages of this formulation.

improving metro rail capacity based on metro demand (see Figure 28). Also, a small percentage is assigned for implementing the pricing scheme itself. The remainder is collected and not spent on activities represented in the model.

Moreover, in order to counter social exclusion issues (such as deprived mobility due to unavailability of transit), the model considers discounts for local residents and the exemption from congestion pricing of disabled residents, similar to the actual implementation of the pricing scheme in London. Also, fleet vehicles within the charging area are assumed to have the same type of privileges and are treated in the same way as the policy makers consider these vehicles for the London Congestion Pricing Scheme. The corresponding data and parameters are described in more detail in Section 5 and Appendix B.

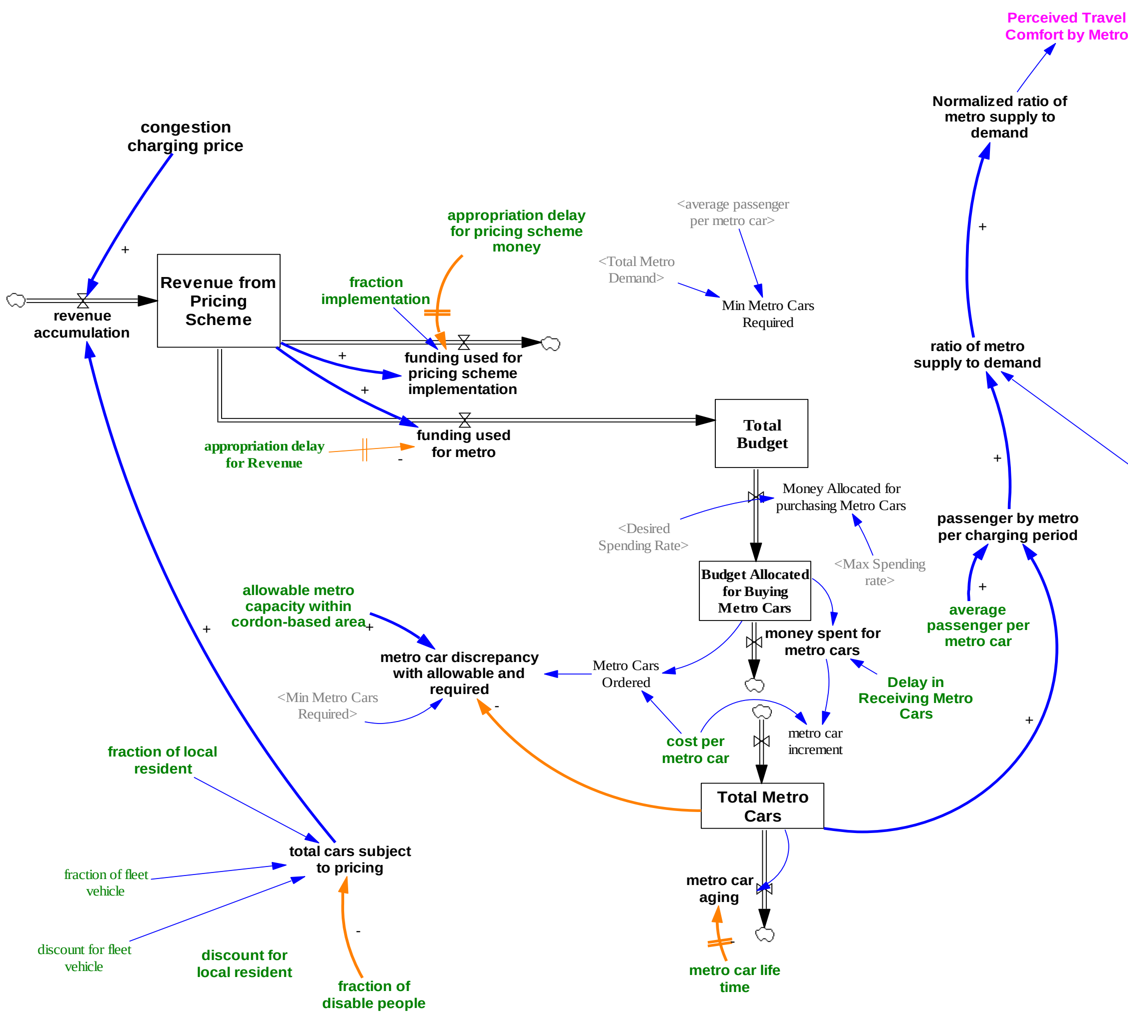

Figure 28- Charging Revenue Distribution and Mass Transit Improvement

In order to represent the changes in the socializing activities of drivers, the variable 'average trip length' is defined in the model (see Figure 29). The impact of driving conditions on the average length that drivers travel (i.e., 'average trip length') is estimated by the 'attractiveness of driving car' set to the power of the parameter 'strength of impact on trip length' and multiplied by the 'maximum trip length'. The data source for 'maximum trip length' is provided in Appendix B. Also in Section 5 we describe how the 'strength of impact on trip length' is found by calibration of the 'average trip length' simulation values against the available data for 'average trip length'. As can be observed in Figure 29, the traffic volume, which is the multiplication of 'average trip length' and 'total car running,' is divided by the highway capacity to determine the 'normalized density on roads'. This variable will determine the 'perceived density on roads', which consequently impacts the 'attractiveness of driving'.

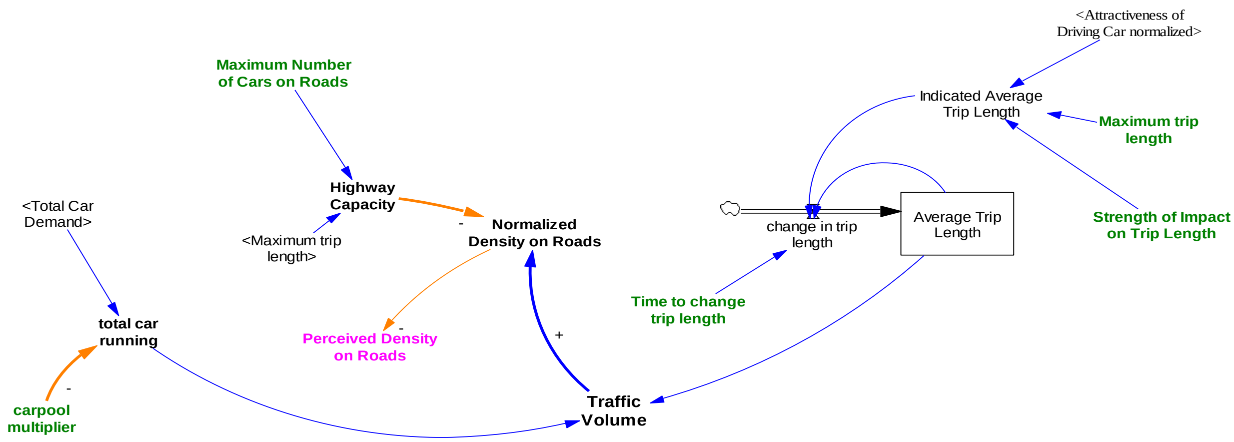

Figure 29- Average Trip Length Change

3.1 The Determination of Equilibrium

The model should be set to equilibrium to separate transient dynamics of the model from systematic dynamics of the model while permitting controlled experimentation (J. Sterman, 2000). In equilibrium, the value of all stocks is constant, meaning that the sum of the inflows and outflows of every stock is zero. We now determine the requirements that put the model in equilibrium. Note that our purpose is to mainly study people's mode selection and switching behavior without any population growth.

In order to find the initial values of different stocks in the model for the equilibrium condition, if the values of 'normalized density on the roads', and the 'normalized ratio of driving cost to budget' for the initial conditions of the simulation are known, then we can evaluate the equilibrium value of the 'attractiveness of driving'. Then, based on the attractiveness of driving, we can calculate the initial number of cars demanded for the model to be in equilibrium. Finally, based on the formulation for the market share for car and metro (equations 2 and 3), the initial metro demand for the equilibrium condition can be calculated. In other words, different scenarios can be determined for setting the model in equilibrium based on the initial values of 'normalized density on the roads', and the 'normalized ratio of driving cost'. In each scenario, initial values for the 'indicated market share for car' and 'indicated market share for metro' are found. If the amount of 'initial car demand' and 'initial metro demand' based on the data, are equal to the determined value for their corresponding indicated market shares for the equilibrium condition of the model, and the total demand does not change due to population growth or tourists entering the zone, then the system would remain in equilibrium throughout the simulation as indicated by the 'Base Run' in Figure 30 and Figure 31.

However, if, for example, the 'initial metro demand' based on the data is less than the indicated market share determined by equilibrium conditions, while the 'initial car demand' data is equal to its equilibrium level, then the switch rate from the car to the metro mode will become positive, while the switch rate from metro to car is set to zero. The switching between modes occurs until a new equilibrium is realized, as indicated by the simulation run 'Less Initial Metro Demand' in Figures 8 and 9. Similarly, when the 'initial metro demand' based on the data is higher than its equilibrium value, then the 'switch rate from metro to car' would become positive and the 'switch rate from car to metro' would be zero. So, some of the metro demand will continue to switch to car mode, until both stocks reach equilibrium. The same holds if we assume the initial metro demand constant and the initial car demand higher or less than equilibrium level (see Figures 8 and 9).

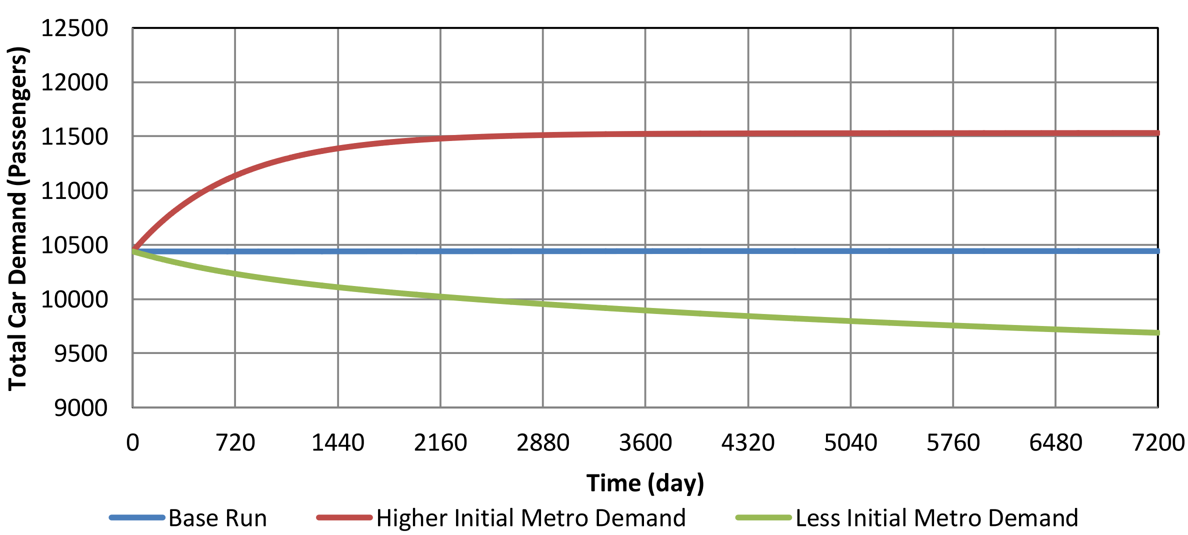

Figure 30- Total Car Demand in Equilibrium

Based on the fact that before the implementation of the pricing scheme in year 2003, London was very congested, so for the initial setting of the model, density on roads should be high and 'perceived density on roads' should have the maximum *high* membership domain. Hence, we postulate that, with the initial car demand of 515,200 passengers in year 2003, the normalized density on roads should initially be equal to 1. In this case, for the initial car demand of 515,200 passengers in London, the corresponding normalized attractiveness of driving a car would be 0, meaning the roads are highly congested. In this condition, equations 2 and 3 would evaluate the initial metro demand as unbounded for the equilibrium condition of the model. Since the total metro demand, in year 2003, in London is 1,275,000 passengers, then according to the structure of the model, the implementation of the pricing scheme would lead to switching from the car to metro mode and hence a decrease in the congestion of the area, until a new equilibrium of the whole system is reached.

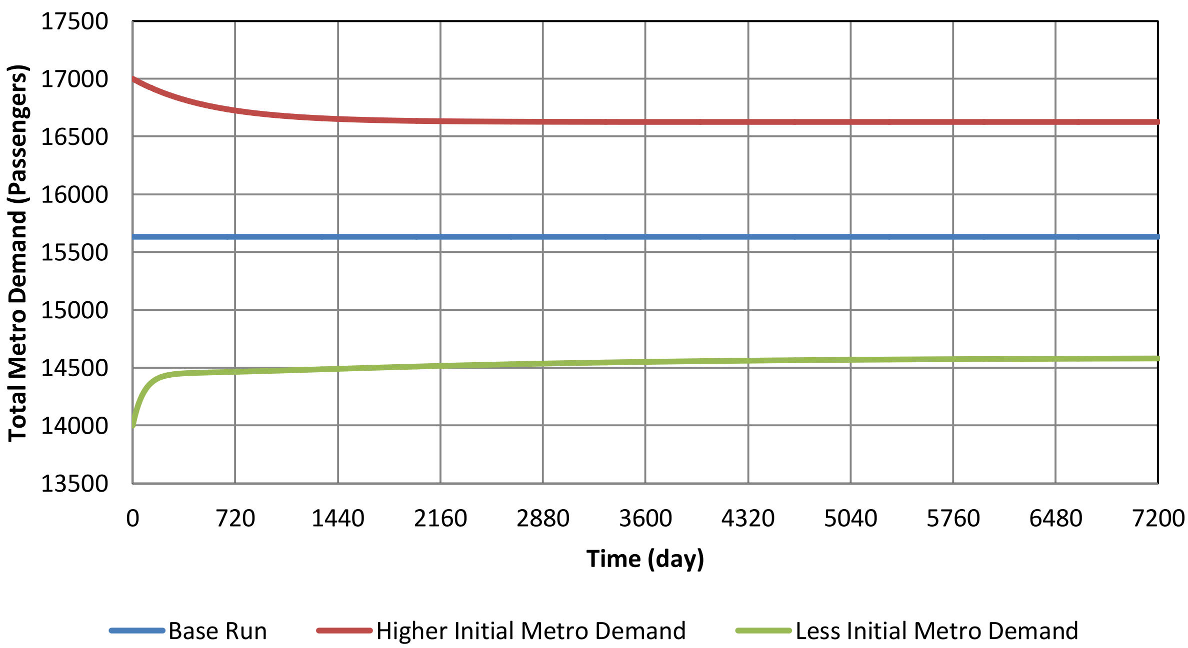

Figure 31- Total Metro Demand in Equilibrium

In addition, the equilibrium level of 'total car demand' and 'total metro demand' also depends on the equilibrium of 'total metro cars' and 'total budget' stocks. For this purpose, 'total budget' available should exceed or be equal to the required budget for maintaining and supplying the metro cars to improve mass transit. The 'total budget' is a function of cost per metro car, metro cars required, metro car life time and delay in receiving metro cars, and the required budget is a function of congestion charging price, total cars subject to pricing and delay in receiving revenue (see Appendix B for details on these parameters and the data sources). So, the equilibrium level of car and metro demand also depends upon all the parameters that determine whether total budget covers the required budget or not, such as cost per metro car and congestion charging price. Some of these parameters are more critical in determining the equilibrium level, which is verified by the sensitivity analysis of the model discussed in Section 3.2. If there is no data available to determine these parameters, then they should be found by calibration.

Depending on the value of these parameters, the initial demand for car and metro for the equilibrium condition will change. If the parameters change somehow, so that the collected revenue does not match the required budget, then the system would no longer be in equilibrium. If later in the simulation sufficient budget could be accumulated to supply the required number of metro cars, then total metro or car demand will switch to the other mode until a new equilibrium emerges. In some extreme cases, metro cars will decrease to close to zero, for which the total metro demand will also fall similarly.

Overall, based on the market share for car and metro travel modes evaluated for the equilibrium condition of the system, and the comparison with the data available for the current condition of the system, we can verify whether the implementation of the pricing scheme is effective or not. The desired market share for each mode is determined based on the relative attractiveness of each mode to other modes and the initial values of metro and car demand (equations 2 and 3). For example, in the case of a very high demand for metro, the relative attractiveness of different modes may indicate a larger market share for cars. So in some situations, even charging drivers for entering the congestion zone will not mitigate the traffic density on the roads, and passengers may still switch to the car mode. This is one of the key conclusions of this analysis. *In general, the comparison of the initial value of metro and car demand is critical in determining the effectiveness of the pricing scheme. If the initial metro demand is higher than a certain value, implementing the congestion pricing scheme will not mitigate any of the traffic congestion.* In other words, even if the revenue is sufficient to improve the alternative transportation mode, the improvement does not necessarily lead to the mitigation of traffic. So premise 2, which states that '*Improvement of alternative transportation modes can have a positive effect on the mitigation of traffic congestion in a cordon-based urban area'*, is a statement of possibility but does not guarantee a positive effect.

Furthermore, the desired market share for the metro mode can only be reached when a sufficient budget could be accumulated to supply the required number of metro cars. Several parameters determine whether this condition is satisfied or not, such as cost per metro car, congestion charging price, and allowable metro capacity within the cordon-based area. The above conclusion links to premise 1. Premise 1, which states that '*Revenues generated from congestion pricing scheme will substantially improve the alternative transportation modes',* is verified depending upon how much revenue is accumulated and whether it is sufficient to cover the cost of improving mass transit and also whether it is available within a reasonable time delay to improve the metro system. If the amount of revenue is not sufficient or is not accessible within a reasonable time delay, then the accumulated revenue will not improve the alternative transportation modes.

3.2 The Model Parameters

In order to determine the values of the model parameters, we need to find out which ones are critical in explaining the model behavior. Hence, a sensitivity test scenario is defined for each parameter. In this sensitivity test we change the parameter values to extreme values and observe whether the model is behaving in a reasonable way or not. Furthermore, additional insights are obtained from each test since we can understand whether the parameter is critical for explaining changes in the resulting model behavior. Additionally, as we discussed in Section 3.1, some parameters of the model, at certain values, may lead to values for the total budget that cannot cover the required budget for maintaining and supplying the metro cars to improve mass transit. If the revenues generated cannot cover the required budget, then the pricing scheme will not significantly improve the alternative transportation mode and therefore will not have real impact on mitigating traffic congestion. This would make the congestion pricing scheme ineffective and should be considered before actually implementing such a scheme. This observation is closely related to premises 1 and 2.

Overall, we can categorize the parameters into three groups. One group of parameters consists of those for which the value is not critical in explaining the behavior of the model. Among the remaining parameters which have significant impact on the behavior of the model, some impact the effectiveness of the pricing scheme. The rest may not impact the scheme but should be studied, because they determine the behavior of the model. After performing the sensitivity analysis, among 26 parameters of the model, the non-critical parameters include the appropriation delay for pricing scheme money, the maximum trip length and the fraction implementation which are found based on data (see Appendix B). Also the sensitivity analysis determines the parameters that impact the effectiveness of the congestion pricing scheme. These are allowable metro capacity within cordon-based area, appropriation delay for revenue, average passenger per metro car, cost per metro car, delay in receiving metro cars, maximum acceptable congestion charge, metro car life time and time for order. Most of these parameters are determined by the data. If there is no data to define the parameters of this category, then they should be determined by calibration as we will discuss in Section 5. Also, further insights from the sensitivity analysis tests are provided in Section 6. The three categories with their respective parameters are presented in Table 3.

Table 3-Categorization of Parameters based on their Critical Impact

Categories of Parameters	Parameters	
Critical in Determining the Behavior of the Model		
	Determined based on Available Data:	**Determined by Calibration:**
Affect the Effectiveness of the Pricing Scheme	- Allowable metro capacity within cordon-based area - Average passenger per metro car, - Cost per metro car, - Delay in Receiving Metro Cars, - Maximum Acceptable Congestion Charge - Metro car life time - Time for Order	- Strength of Impact on Trip Length - Time to change trip length - Time with car before switching - Time with metro before switching
Does not Affect the Effectiveness of the Pricing Scheme		- Appropriation delay for Revenue
Not Critical in Determining the Behavior of the Model		
	Determined based on Available Data:	
	- Fraction implementation - Maximum trip length - Appropriation delay for pricing scheme money	

4. Overview of Data and Information

This research is based on data available from the congestion pricing policy implemented within the London metropolitan area which is freely available at the Transport for London website (TFL, 2011b). The parameters of the model are determined based on data collected from London Pricing Scheme implemented in year 2003. So, the starting point for the simulation is the beginning of year 2003. However the initial values for 'total car demand' and 'total metro demand' belong to year 2002, before the congestion pricing scheme was implemented.

Based on the London congestion charging scheme data (TFL, 2006), the congestion price is assumed to have a constant value of £5 until July 2005, and then £8 for the remainder of the simulation.[12] Traffic for London (TFL, 2006) expected that this increase would result in further reduction in traffic entering and circulating the charging zone and in reduction in delays within

12 So in order to include the increase of the congestion charging price, a step function is used which adds £3 to the 'congestion charging price' at beginning of July year 2005 (i.e., 5+STEP(3,942)).

the charging zone, and also result in additional net revenues.[13] Regarding the metro system, we only consider the London Underground Limited (LUL) and not the Dockland Light Railway (DLR), since total metro demand data is only available for LUL. Also, since the data regarding LUL metro cars and passengers using LUL is for the whole LUL system, we consider the whole LUL as the metro system, even though not all parts are in the congestion charging zone area. A full description of the parameters and their data sources is provided in Appendix B.

5. Calibration

5.1 Selection of variables and parameters

According to the Traffic for London reports (TFL, 2004, 2005, 2006, 2007a, 2007b, 2008, 2009), time-series data are available for several of the variables in the model. For example, based on Table B.2 (see Appendix B), we can estimate the 'total metro cars' running in the London Underground each year, which is summarized in Table 4.

Table 4- Total Metro Cars

Year	Cars
2000	4066
2001	4066
2002	4066
2003	4066
2004	4066
2005	4066
2006	4066
2007	4066
2008	4066
2009	4066
2010	5321

The 'total car demand' is calculated based on the traffic entering the central London charging zone during charging hours, based on the Impact Monitoring-Fifth Annual Report (TFL, 2007a),(Table 2-2, p.22). Also by using the year-to-year changes in traffic figures over the years, and multiplying by the carpool multiplier for cars and minicabs found in London Travel Report (TFL, 2007b), (Table 1.3.2, p.6), the van multiplier (assumed equal to 4) and the lorry multiplier (assumed equal to 2), we calculate the number of 'total car demand' by passengers, over time (see Table 5).

[13] According to the implementation of this pricing scheme, there was an increase to the original boundary of the congestion charging zone in Feb. 2007 by the westbound extension. However, we do not consider this extension, because currently policy makers are considering removing the westbound extension (BBC, 2008).

Table 5-People entering central London during charging hours (000's)

Year	2002	2003	2004	2005	2006
Car Multiplier	1.36	1.35	1.37	1.39	1.38
Van Multiplier	4	4	4	4	4
Lorry Multiplier	2	2	2	2	2
Cars	265.2	175.5	176.319	173.75	172.5
Vans	220	196	194.04	188.16	192
Lorries	30	26	24.7	24.44	26
Total Chargeable Cars	**515.2**	**397.5**	**395.059**	**386.35**	**390.5**

The 'total metro demand' is calculated based on the "passengers exiting LUL stations in and around the charging zone" during charging hours from the Impacts Monitoring Reports on the Traffic For London website (TFL, 2006, 2007a). The numbers for years 2002 to 2005 were found in the Impacts Monitoring-Fourth Annual Report (TFL, 2006) (p. 63) and for year 2006 it was found in the Impacts Monitoring-Fifth Annual Report (TFL, 2007a) (p.62) (see Table 6).

Table 6- Total Metro Demand

Year	Metro Passenger
2002	**1,275,000**
2003	**1,258,500**[14]
2004	**1,247,000**
2005	**1,226,000**
2006	**1,286,000**

The initial value for 'total metro demand' and 'total car demand' is considered to be the value for year 2002, i.e., 1,275,000 passengers for metro and 515,200 passengers for cars. The data shows that the sum of 'total car demand' (passengers) and 'total metro demand' (passengers) over the years is not constant (see Table 7)[15]. The reason is that some of the demand switched to other travel modes including bus, or switched to using bicycles and trails to commute to work. On the other hand, in our model, we assume that the sum of total car and metro demand is constant. So, in the model, if the total car demand decreases in the model, consequently the total metro demand should increase because the car drivers can only switch to metro demand other than car. In order to make a reasonable calibration against the available data, we have to

[14] Since we want to avoid including the exogenous effect of the temporary but prolonged closure of the Central Line, the transfer of passengers to buses and a general decline in tourism, we substitute the original value of 1,181,000 with the average of the total metro demand over years 2002, 2004, 2005 and 2006.

[15] The unit for 'Total Car Demand' is in passengers, not divided by the average carpool multiplier, so that we can easily compare and add with 'Total Metro Demand' which has the same unit of passengers.

either choose to calibrate against total car demand data or total metro demand data. Since a major objective of the model is to study the mitigation of road traffic, and according to data, changes in car demand are more significant, in calibration we only regard the changes of total car demand, and total metro demand changes are not considered in the calibration.

Table 7-Sum of Total car and Total Metro Demand

Time	0	365	730	1095	1460
Total Car Demand + Total Metro Demand	1,790,200	1,656,000	1,642,059	1,612,350	1,676,500

With respect to the 'average trip miles' (mile/person/day), the data is estimated by converting the kilometer values in Table 8 to mileage values. Also the value in year 2003 is assumed equal to average trip miles in 2001 (i.e., 12.3 km., or 7.64 mile) and the values in years 2005 to 2008 are all assumed equal to 12.0 km. (i.e., 7.46 mile) per person per weekday. The table has been documented in the Travel in London-Key Trends and Developments: Report Number 1 (TFL, 2009) (Table 9.6, p. 147). Our focus is Central London, as shown in Table 8.

Table 8-Average Trip Miles per Person per Day (km) by Area or Region of Residence (TFL, 2009)

Area of Residence	Average Weekday		2005-2008 Average			
	1991	2001	Weekday	Saturday	Sunday	All days
Central London	11.5	12.3	12.0	10.6	12.2	11.8

For the total 'revenue from the congestion pricing scheme', the total congestion charge payments from non-local residents is summed up and the penalty charges or enforcement income is excluded, over the financial years 2004 to 2007 based on Impacts Monitoring Annual Report by Transport for London (TFL, 2005, 2006, 2007a) (see Table 9). In order to use this data series for calibration, we need to accumulate the number over the years and use 115, 255 and 407 Million Pounds, so that it matches with the stock variable, 'revenue from pricing scheme', defined in the model.

Table 9-Revenue from Congestion Charge

Financial Year	Revenue (Million Pound)[16]
2004/2005	**115**
2005/2006	**140**
2006/2007	**152**

To make the model consistent with the available data, some parameter values need to be calibrated. The selection of these parameters largely depends on the sensitivity analysis results. As discussed in Section 3.2, the 'strength of impact on trip length' and the 'time to change trip

[16] This is the sum of standard daily vehicle charges plus fleet vehicle daily charges.

length', 'time with car before switching' and the 'time with metro before switching' have a critical effect on the model behavior. However, there is no data to determine the value of these parameters. So these variables need to be calibrated to match the following variables against their respective time-series data, 'average trip length', 'total car demand', 'total metro cars' and 'total revenue' accumulated.

5.2 Results and Insights from the Calibration

After performing the calibration, we observe that premise 3, which states that '*A congestion pricing scheme cannot effectively resolve congestion problems in short term due to the existence of delays'* is not fully valid. The calibration process matches the behavior of the model to data, and so we observe that the pricing scheme can mitigate traffic congestion initially. However, the impact is less effective later on, and does not further decrease the congestion level; however it maintains it at a lower level when compared to before implementing the scheme.

We ran the calibration for a number of iterations by considering the 'strength of impact on trip length', 'time to change trip length', 'time with car before switching', 'time with metro before switching' and 'appropriation delay for revenue' parameters. However, based on the conditions, only the switching from car to metro mode occurs and the switching from metro to car mode is zero. Therefore, we exclude the parameter 'time with metro before switching', because it is not affecting the results, and run the calibration again. In each iteration of the calibration, the objective function is minimized, which is equal to the sum of differences between the time-series data of 'average trip length' (ATL), 'total car demand' (TCD), 'total metro cars' (TMC) and 'total revenue accumulated' (R) and their respective simulated values, multiplied by the weight specified and then squared as in equation 5.

$$Minimize\left(\int_{t=Year\ 2003}^{Year\ 2012}\left(\left(w_1\left(ATL(t)-ATL_{data}(t)\right)\right)^2+\left(w_2\left(TCD(t)-TCD_{data}(t)\right)\right)^2+\left(w_3\left(TMC(t)-TMC_{data}(t)\right)\right)^2+\left(w_4\left(R(t)-R_{data}(t)\right)\right)^2\right)\right) \quad (5)$$

The weights considered are the reciprocal of the standard deviation of the prediction error for that variable, converging to the maximum likelihood values of the parameters, but under the condition that error terms are normally distributed (Greene, 1997; Vensim, 2010). The initial weights for the first iteration for each variable are considered equal to the reciprocal of the standard deviation of the time-series data for that variable. The changes in the weights for all the four variables are negligible from the second to the third round, so we stopped at the third iteration (see Table 10).

Table 10- Changes in the Weights between Iterations

Variable/Iteration	Iteration 0	Iteration 1	Iteration 2	Iteration 3
Total Car Demand	2.02889E-05	3.12542E-05	3.17051E-05	3.17111E-05
Total Metro Cars	0.002535443	0.003038166	0.00303257	0.003032492
Revenue	1.84697E-08	9.97881E-09	9.99443E-09	9.99461E-09
Average Trip Length	13.4112	41.01988983	42.10448074	42.11997986

The parameter values found after the final iteration of calibration and further details are shown in Table 11. In total there were 30 restarts for the final iteration and 7 unique local optima were found. Among all restarts, 40% found the same local optima reported as the one with the lowest payoff function value (see Table 11). The comparison of the data with the variables calibrated is shown in Figure 32 to Figure 36.

Table 11- Calibration Results for the third iteration without Total Metro Demand Data

Payoff Function	-17.4886
No. Simulations	8474
Parameter	Value
Time with car before switching	2657.68
Time to change trip length	869.584
Strength of Impact on Trip Length	0.0110058
Appropriation delay for Revenue	168.115

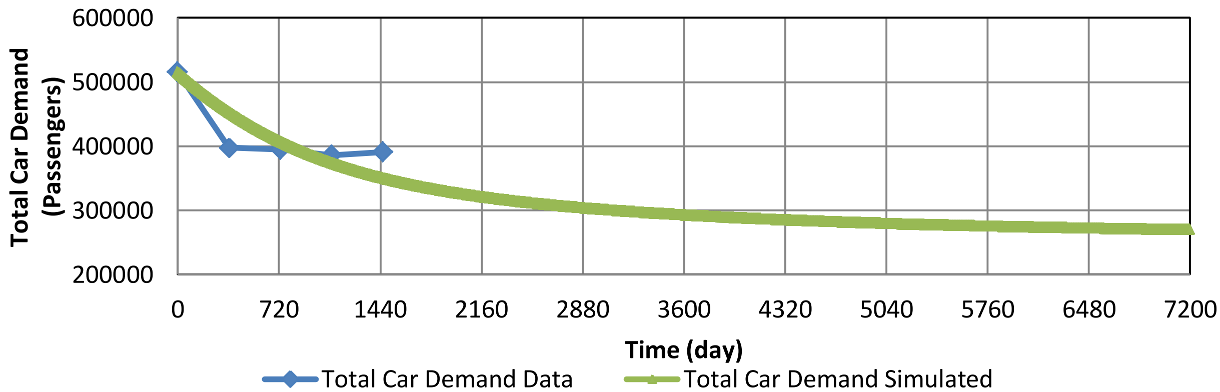

Figure 32- Total Car Demand, Data vs. Simulated Values

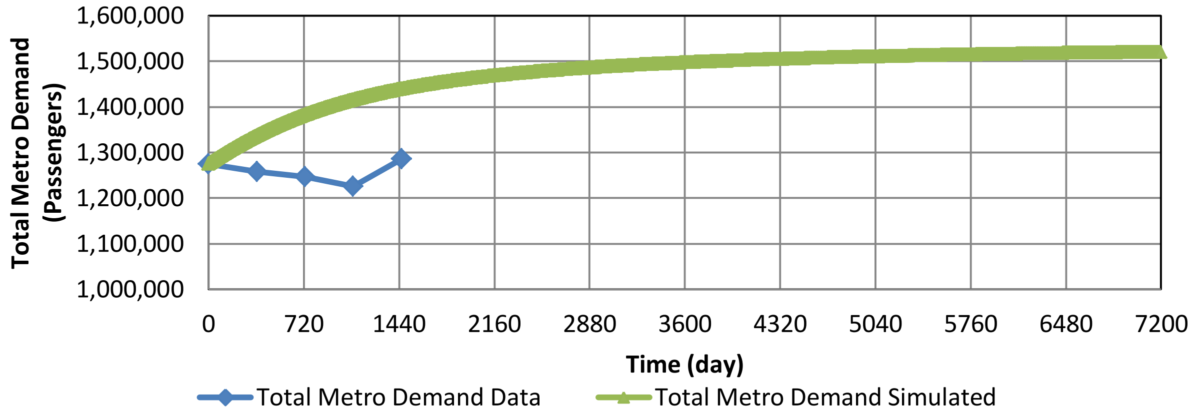

Figure 33- Total Metro Demand, Data vs. Simulated Values

Based on the calibration results, the 'total car demand' matches the data as expected. The car demand decreases significantly in the initial phase of the implementation of the pricing scheme and then levels out further on in the future, meaning that the pricing scheme cannot be effective in mitigating the traffic congestion for an unlimited period of time. With respect to the 'total metro demand', as we discussed earlier in Section 5.1, and Table 8, since the model does not consider other modes of travel, it cannot capture the decreasing behavior of 'total metro demand'. The simulation results indicate that passengers switch to an alternative travel mode, other than driving a car.

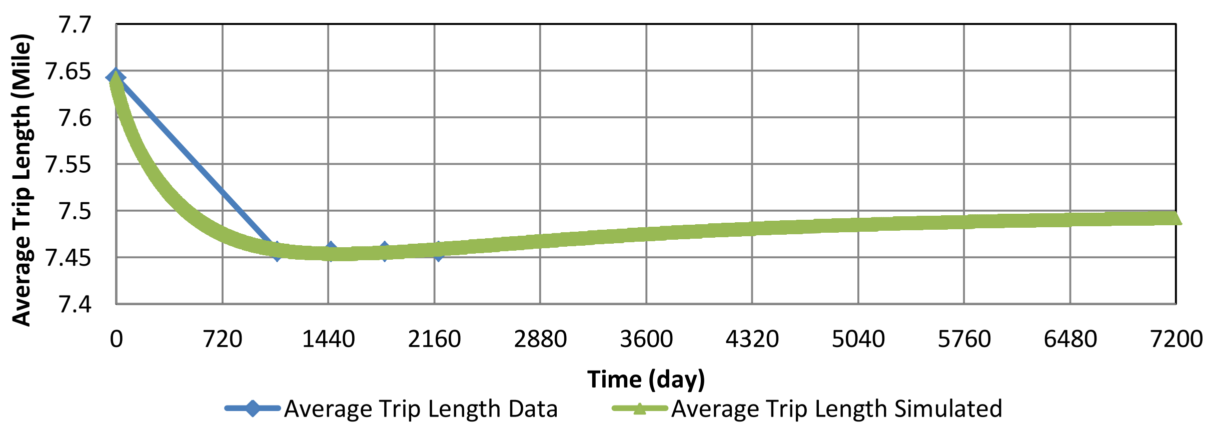

Figure 34- Average Trip Length, Data vs. Simulated Values

As shown by the calibration results, the 'average trip length' is decreasing initially, which matches the data, due to the decrease of the car demand, but as the congestion on the roads decreases and consequently the 'attractiveness of driving' increases, then drivers are able to travel longer distances, and the 'average trip length' increases over time (see Figure 34).

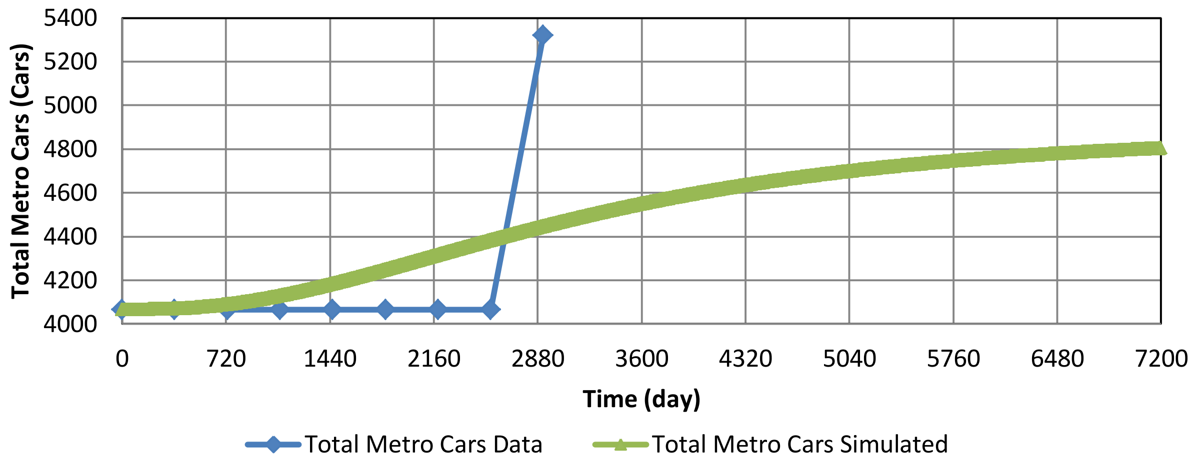

Figure 35- Total Metro Cars, Data vs. Simulated Values

The implementation of the congestion pricing scheme generates revenue that is spent for buying extra metro cars. In the simulation model, the increase of metro cars has an S-shaped growth (see Figure 35), meaning that growth is exponential at first, due to the dominance of the reinforcing loop "R3-higher attractiveness of riding metro-higher supply of metro cars" (see Figure 23). Then, gradually, due to the dominance of the balancing loop "B5-Closing the gap between current available and required metro cars" the growth slows down until it reaches the equilibrium level of 'minimum metro cars required'. However, according to the available data, a new batch of metro cars is bought in 2009, which causes a sudden increase in the number of metro cars (Table B.2, Appendix B). This makes the data trend differ from the simulation results, but both show increasing behavior (see Figure 35). On the other hand, due to 'delay in receiving the metro cars' orders, after ordering the minimum metro cars required, only 0.9340 of the required metro cars would be running in the system and the remainder are in the ordering pipeline. Thus the simulated values of 'total metro cars' are less than the data values (see Figure 35).

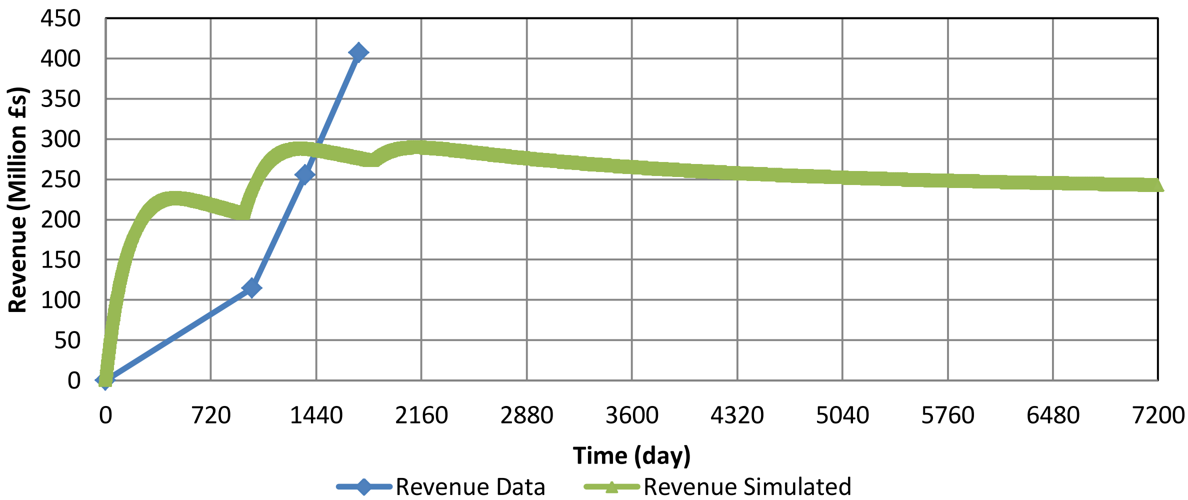

Figure 36- Revenue, Data vs. Simulated Values

According to Figure 36, the revenue values have two jumps during the simulation. At July 2005 (i.e., 942 days), due to an increase in the daily charges in from £5 to £8 for standard vehicles and from £5.5 to £7 for fleet vehicles, the revenue values have a sudden increase. Then, at the end of year 2008 (i.e., 1825 days), revenue is no longer spent for implementing the pricing scheme, and so the simulated values have another sudden increase. Since the data collected for revenue does not capture the amount spent for implementing the scheme, some difference is observed with the simulated values. Overall simulated values decrease due to decline of the number of cars entering the charging zone, according to both data and the simulation results (see also Figure 32).

6. Sensitivity Analysis and Behavioral-Policy Insights

According to the results, if the initial number of metro cars is not sufficient to provide service for the metro demand, then an extreme high value of the parameter 'appropriation delay for revenue' (i.e., 20,000 days), would result in an insufficient budget to supply the required number of metro cars. In this situation, the car demand will switch to metro mode with a higher delay and consequently it will take much longer for the scheme to be effective in mitigating traffic congestion even if the roads are highly congested (see Figure 37). In other words, only in this extreme case, the parameter, 'appropriation delay for revenue', is critical to determining the effectiveness of the pricing scheme. Under normal conditions, we assumed the value of the parameter to be one month (i.e., 30 days).

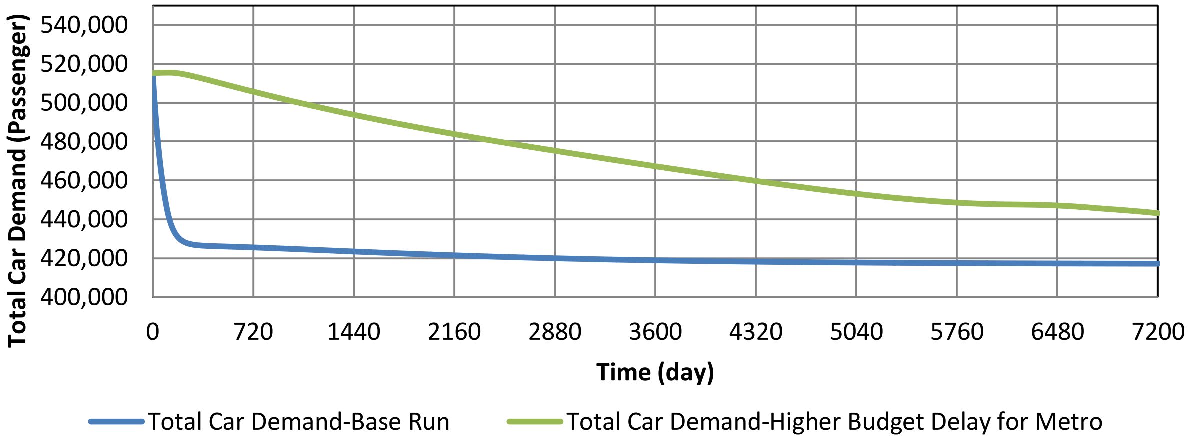

Figure 37- Total Car Demand with Higher Budget Delay (i.e., 20,000 days) for Metro

Based on the sensitivity test, the parameter 'cost per metro car' is critical in the sense that if it is too high (i.e., 7.5e+030 £s/metro car compared to the base case of £750,000/metro car), so that there is not enough budget collected to buy the required metro cars, then the pricing scheme will not be effective. In other words, the metro demand will switch to car mode and congestion will even get even worse (see Figure 38).

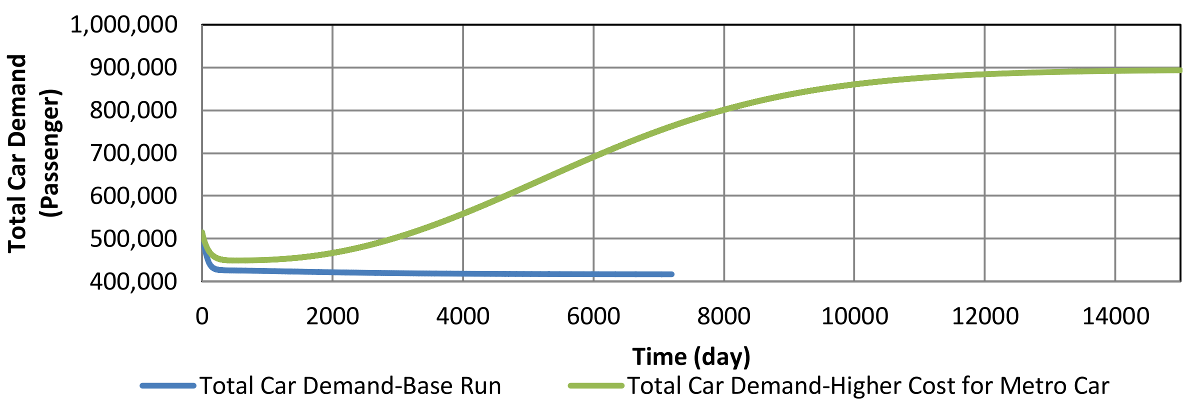

Figure 38- Total Car Demand with higher cost for metro car (i.e., 7.5e+030 £s/metro car)

Moreover, if the parameter 'delay in receiving metro' is higher (i.e., 5,000 days or 10,000 days), than the base case of 1095 days, then the car demand will not decrease as much as the base case and the pricing scheme will not be effective as required (see Figure 39).

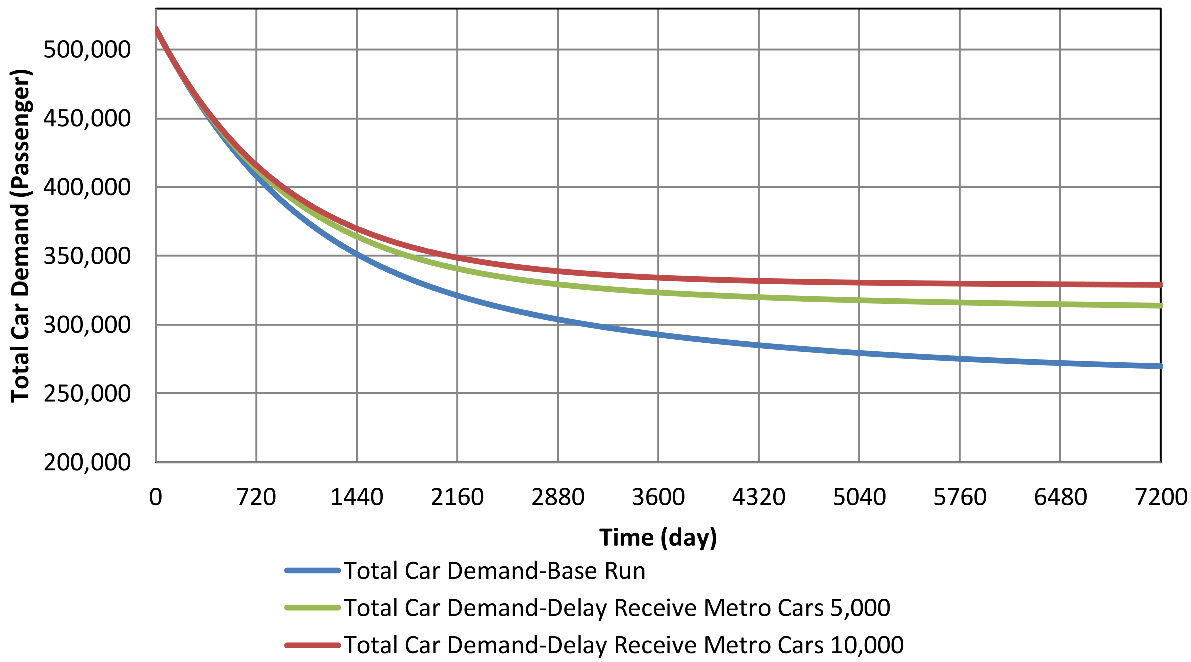

Figure 39- Total Car Demand with Higher Delay in Receiving Metro Cars (i.e., 5,000 or 10,000 days)

There are no data to determine the parameter 'maximum acceptable congestion charge'. It is reasonable to assume it is equal to the initial congestion charge, when the scheme is implemented. However, based on the sensitivity analysis, it is understood that if the parameter is increased over the years, for example, if the 'maximum acceptable congestion charge' increases to £8 at 940 days (i.e., 2.6 years), meaning that people do not regard the initial congestion charging cost as high as initially perceived, then the pricing scheme will lose its effectiveness over time and the congestion on the roads will rise to the original value, unless the policy makers increase the charging cost according to the increase of maximum acceptable congestion charge. This is very critical for the policy makers to consider (see Figure 40).

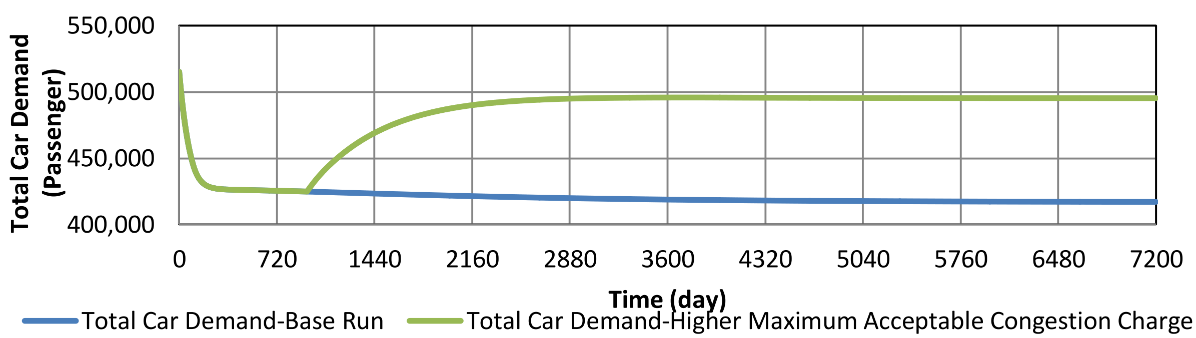

Figure 40- Total Car Demand when Maximum Acceptable Congestion Cost increases to £8 at 940 days (i.e., 2.6) years

Some of the parameters are found based on data that are already described in Section 5. The rest of the parameters including 'strength of impact on trip length', 'time to change trip length', 'time with car before switching' and 'time with metro before switching' are found by calibrating the model against data, as discussed in Section 5.2.

6.1 Analysis of Behavioral Impacts

In the model, we assume that average trip length represents the socializing activities of passengers, and if passengers engage more in socializing activities, then they will travel longer distances. The available data from London verifies our assumption. According to the third annual report (TFL, 2005) for the Congestion Pricing Scheme implementation in London Cordon area, some activities undertaken by car have been shown to increase after the implementation of the charging scheme, while simultaneously congestion levels have decreased (see Table 5). These activities include main food shopping (1% increase), visiting friends/family (1% increase), non-food shopping trip (3% increase) and any leisure trip (1% increase) (see Table 12).

Furthermore, the data supports that an increase in leisure trips took place from year 2006-2007 to 2007-2008. According to Report Number 1 by Transport for London in describing key trends and developments (TFL, 2009), a "slight fall in the share of commuting trips . . . with a corresponding increase in the share of leisure trips" (p. 148) is observed (see Table 13).

Table 12- Activities Undertaken by Car for Socializing Trips, during Charging Hours, within the Charging Zone (TFL, 2005)

	Charging Zone Respondents			Inner London Respondents		
	Before Charging (2002)	After Charging (2003)	+ / -	Before Charging (2002)	After Charging (2003)	+ / -
Base (all panel)	430	430		678	678	
Main food shopping	20%	21%	+ 1 %	13%	8%	- 5 %
Commuted to and from work	17%	14%	- 3 %	12%	9%	- 3 %
Visited friends/family	16%	17%	+ 1 %	10%	6%	- 4 %
Any health trips	12%	8%	- 4 %	9%	7%	- 2 %
Any business trips	10%	5%	- 5 %	8%	5%	- 3 %
Non-food shopping trip	10%	13%	+ 3 %	5%	3%	- 2 %
Any leisure trip	9%	10%	+ 1 %	3%	3%	0 %
Trip for services or facilities	9%	7%	- 2 %	3%	2%	- 1 %
Escorted to/from school/nursery	9%	6%	- 3 %	2%	1%	- 1 %
To and from school/college	3%	2%	- 1 %	1%	1%	0 %
Any Activity	42%	38%	- 4 %	37%	24%	- 13 %

Table 13- Percentage Shares of Travel Distance by Trip Purpose, Average Day, 2006/07 and 2007/08, 7-day week (TFL, 2009)

Trip Purpose	Distance per person (kms)		Percentage of travel distance	
	2006/07	2007/08	2006/07	2007/08
Commuting	3.5	3.2	23%	22%
Other work	2.1	2.2	14%	15%
Education	0.8	0.6	5%	4%
Shopping and personal business	2.7	2.6	18%	18%
Leisure	4.7	5.0	31%	33%
Other	1.2	1.2	8%	9%
All purposes	15.0	14.9	100%	100%

On the other hand, surveys show an opposite result for the western extension of the pricing scheme in London. According to the survey results which are reported in the sixth annual impacts monitoring report (TFL, 2008), “Respondents were most likely to have either reduced their car travel for social and leisure trips or to have changed to a different mode of transport for these trips” (p.134). Also 6% had reduced the frequency of trips to visit friends and family in the extended zone during those hours. These negative outcomes may have contributed to the majority vote to remove the western extension (BBC, 2008). The last day to charge drivers entering the Western Extension was on Christmas Eve, 24 December 2010 (TFL, 2010).

In order to further analyze the behavioral impacts of implementing the pricing scheme, we study the behavior of ‘average trip length’. For this purpose, we knock out certain loops that we hypothesize are responsible for the observed behavior of ‘average trip length’ and we create switches to shut the loop(s) down. In the base case simulation, the ‘average trip length’ initially decreases, and stays constant for some time and then starts to increase as the density on roads decreases and consequently the ‘attractiveness of driving’ increases (see Figure 34). However if we knockout loop B7 indicating ‘higher congestion leads to less average trip length’ (see Figure 41), then the resulting simulation should show that the ‘average trip length’ does not increase the same as in the base case. For this purpose, the effect of ‘attractiveness of driving’ on ‘average trip length’ is made constant at time 150 days (See Appendix C for the link that is frozen to shutdown loop B7.) Compared with the base case, the ‘average trip length’ does not increase as before (see Figure 42).

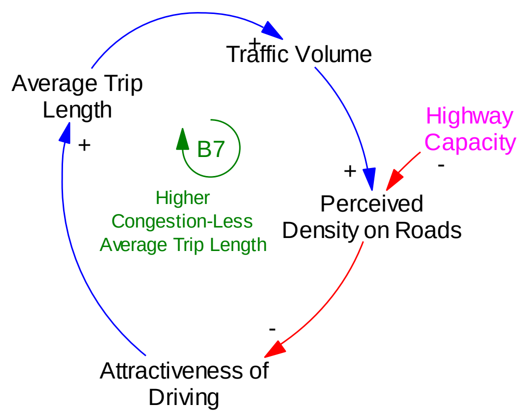

Figure 41- Loop B7-Higher Congestion-Less Average Trip Length

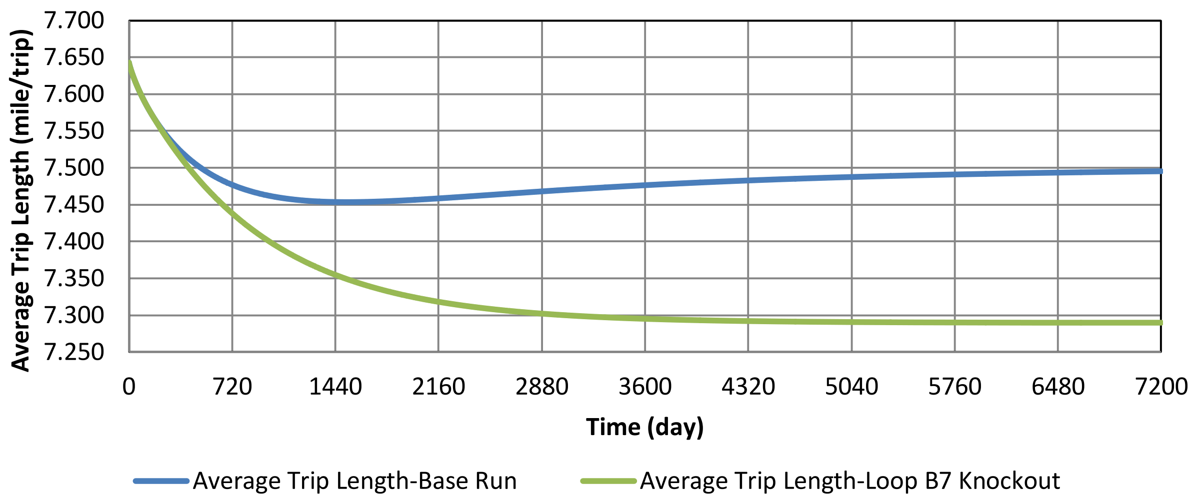

Figure 42- Loop B7 knockout-Change in Average Trip Length

In other words, trip length, which constitutes a major role in social networking is mostly affected by 'attractiveness of driving'. Also, 'attractiveness of driving' is increased by more car passengers switching to metro and so decreasing the density on roads. This is a result of improving the metro transit and buying more metro cars by using the revenue generated from the pricing scheme. In summary, if the metro transit system is improved by increasing the number of metro cars, then car passengers will switch to metro mode which will increase the attractiveness of driving and subsequently passengers will travel longer distances and interact more in social activities.

In order to test whether changes in congestion level are mainly affecting the 'attractiveness of driving' or not, we knock out the different loops by freezing the corresponding links (see Appendix C for the links that are frozen). Then, by comparing all the results, we will find out which loops are the main reason for the increase in 'attractiveness of driving' (see Figure 43).

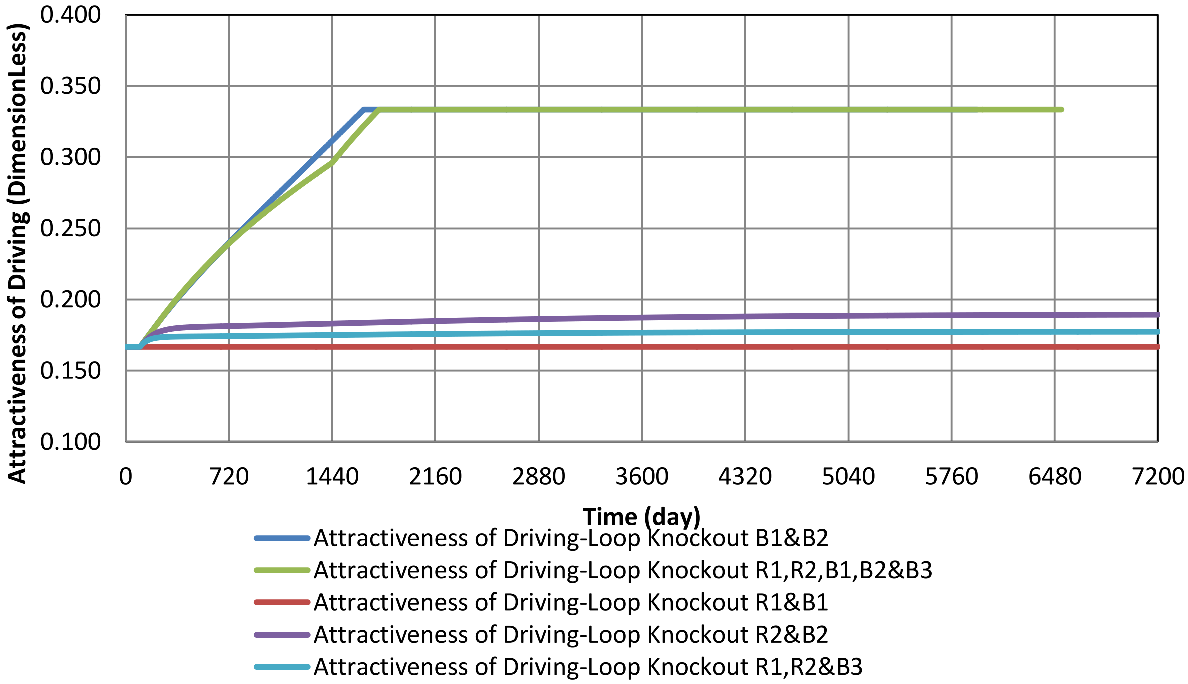

Figure 43- Loops B1, B2, B3, R1, R2 knockout-Change in Attractiveness of Driving

As it turns out in the results, loops R1 (Higher Congestion-More Switching between Modes) and B1 (Higher Congestion-Less Attractiveness of Driving) are mainly affecting the increase of 'Attractiveness of Driving' (see Figure 44).

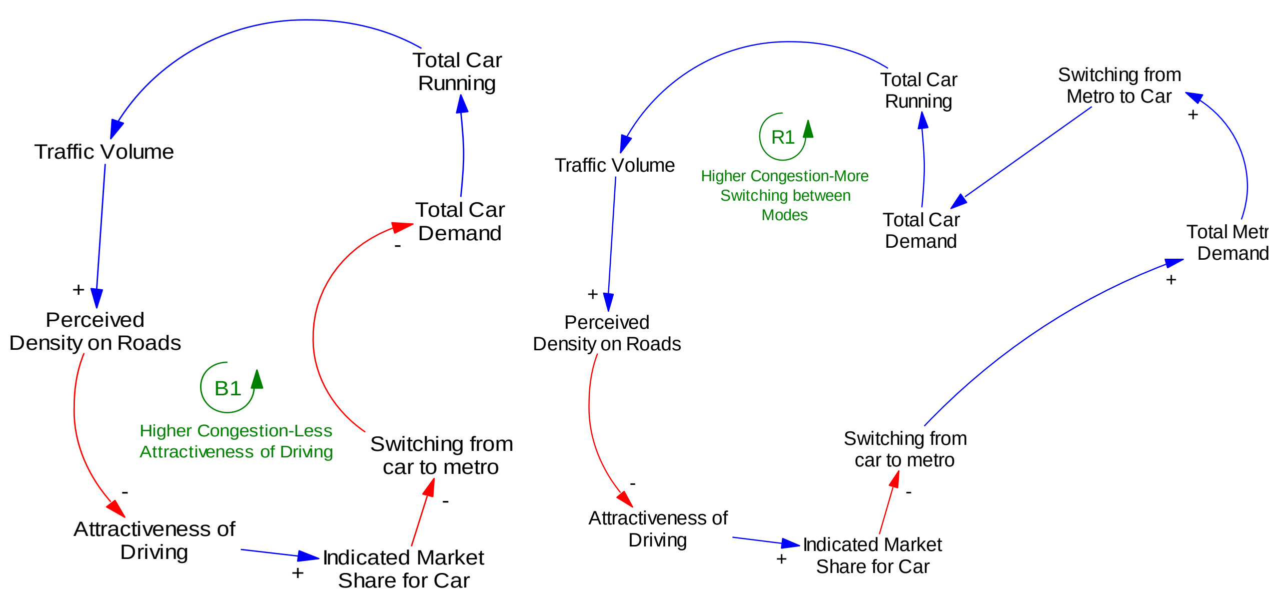

Figure 44- Loop B1- 'Higher Congestion, Less Attractiveness of Driving' and Loop R1- 'Higher Congestion-More Switching between Modes'

If these two loops are knocked out, then, 'attractiveness of driving' does not increase and remains constant. In other words, the main cause associated with increases in 'attractiveness of driving' is congestion mitigation, which then leads to an increase of the 'average trip length' and socializing activities. The mitigation of the congestion on roads occurs because of switching of some of car demand to traveling by metro due to improvement of metro service.

7. Conclusions and Future Research

In this paper, a comprehensive policy analysis is performed to investigate the combinations of key policy variables that would realize the desired traffic congestion mitigation through congestion pricing policy plus the improvement of mass transit capacity. Overall, based on the market share for car and metro travel modes evaluated for the equilibrium condition of the system, and the comparison with the data available for the current condition of the system, we can verify whether the implementation of the pricing scheme is effective or not. In other words, '*Improvement of alternative transportation modes can have a positive effect on the mitigation of traffic congestion in a cordon-based urban area'* (Premise 2) does not guarantee a positive effect for all conditions.

Furthermore, whether '*Revenues generated from congestion pricing scheme will substantially improve the alternative transportation modes'* (Premise 1) or not, is verified depending upon how much revenue is accumulated and whether it is sufficient to cover the cost of improving mass transit and also whether it is available within reasonable time delay to improve the metro system. If the amount of revenue is not sufficient or is not accessible within a reasonable time delay, then the accumulated revenue will not improve the alternative transportation modes.

On the other hand, it is not totally valid that '*a congestion pricing scheme cannot effectively resolve congestion problems in short term due to the existence of all kinds of delays*' (Premise 3). According to the simulation results, a congestion pricing scheme can effectively resolve congestion problems in short term, but cannot be used as a policy to mitigate congestion in the long term (forever). If metro demand increases to a higher value than an indicated market share, then it would eventually eliminate the mitigation of traffic congestion and even lead to increase of car demand.

Another major finding is that the results verify that after the implementation of the pricing scheme, as the density on the roads drops and consequently the attractiveness of driving increases, the 'average trip length' starts to increase. According to the behavioral analysis of the pricing scheme, if we assume that 'average trip length' also represents the socializing activities, then the increase of trip length could potentially represent the reinforcement of the social networks. Expanding this part of the model could be a proposed research project for the future.

Overall, the developed model can be used as a management flight simulator to evaluate various travel demand management strategies and/or their combinations. Consequently, we can determine the proper policies and best values for critical parameters including allowable metro capacity within cordon-based area, congestion charging price, and different discount factors.

There are a number of future directions associated with this research. One direction is to expand the scale of this model to evaluate congestion pricing's impact on environment, land use, the local economy, population dynamics, and the concepts of sustainability and resilience of a metropolitan area to extreme events. Another direction is to do an in-depth analysis once several linguistic variables are integrated in this transportation system dynamics model. One would need to identify the fuzzy rules whenever appropriate data are available. However, this would require some combination of expert opinion elicitation, interviews, survey data, and comprehensive group modeling exercises. This may require adopting different fuzzy membership functions other than the triangular membership function used in this model.

Another important issue is the incorporation of delays in the model, from when a change occurs in the transportation system to the time the perceptions change. In the current model, we assume that changes in conditions of travel by car or metro have an immediate impact on perceptions. However, due to information delay, it will take longer for people to observe the condition and then change their perceptions. Also, the current model does not differentiate between work-trips and non-work trips, which could also be considered in future extension of the model. Another expansion of the model could be with respect to changing the boundaries of the congestion zone or changing the number of charging hours on the traffic demand.

Furthermore, the trip generation part of the model only focuses on populations and social interactions and does not include land use, retail employment, non-retail employment, or residential density. Including socio-economic factors in the trip generation sub-model could be a further expansion of the sociability part of the model. Another extension is improving the representation of the measure of congestion, for example, by including the relationship between speed and congestion, which currently is measured by the density of car volume on the roads.

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Appendix A

An alternative for finding the indicated market shares for car (I_{Car}) and metro (I_{Metro}), is proposed by Ben-Akiva and Lerman (1985) which is to use the common discrete choice models applied in the transportation literature, specifically logit model shown below respectively for car and metro modes.

$$I_{Car} = \frac{e^{A_{Car}}}{e^{A_{Car}} + e^{A_{Metro}}} \times Total\ Demand$$

and

$$I_{Metro} = \frac{e^{A_{Metro}}}{e^{A_{Car}} + e^{A_{Metro}}} \times Total\ Demand$$

However, Dell'Orco and Kikuchi (2004) describe that in the above approach, it is assumed that the attractiveness values A_{Car} and A_{Metro} , include a random term which are presumed to be independent and identically distributed (IID). Also they mention that "only the expected values are known for the attributes associated with each alternative" (p.4). The authors argue that based on such assumption, "it is perhaps reasonable to assume that the uncertainty associated with the utility is the same among alternatives and hence, the assumption of IID property may be upheld" (p. 4).

Nevertheless, as Dell'Orco and Kikuchi (2004) argue, similar to our case, different attributes including the cost of driving, congestion on the roads, and metro comfort of different travel mode alternatives "harbor different patterns of variations" (p.4), which in this case, the vagueness inherent in decision maker's perception of the travel mode condition "is not compatible to the concept of IID" in the aforementioned approach. The authors also conclude from this argument that "from a theoretical point of view, logit model in the form of above equations cannot adequately deal with situations which the variances of the attributes are different" and propose the use of possibility theory to compare the utilities of different alternatives in such situation.

Appendix B- Parameters and Data and Sources

1) Average passenger per metro car

In respect to metro supply in the model, additional metro cars are ordered by estimating the minimum number of metro cars required to supply the total metro demand. According to Travel in London-Key Trends and Developments: Report Number 1 (TFL, 2009), "Train occupancy rates on LU have been broadly constant over the review period, despite substantially increased patronage" (p. 86). Furthermore, the report (TFL, 2009) describes that "increased service provision is generally keeping pace with increased demand as well as contributing to it"(p. 86).

So, we need to estimate the number of required metro cars that pertain to a 100% ratio of metro supply to demand. For this purpose, the parameter 'average passenger per metro car' is defined as the average number of passengers riding metro during the charging hours in a weekday. This is different from the average train occupancy rate already available in Traffic for London report (TFL, 2009), because it is not clear that the numbers reported also include weekends or not. The parameter 'average passenger per metro car' is calculated by dividing the initial value of 'total metro demand', (i.e. 1,275,000 passengers) over initial number of 'total metro cars' (i.e. 4066 metro cars) in year 2002. This is equal to 313.6 and is kept constant throughout the simulation, due to the fact that train occupancy rate has been mostly constant in London (TFL, 2009).

However, due to 'delay in receiving the metro cars' orders, after ordering the minimum metro cars required, only 0.9340 of the required metro cars would be running in the system and the remainder are in the ordering pipeline (See Figure 28). So in order to make the initial metro cars equal to initial metro cars required (i.e. 4066 metro cars), we need to set the value of 'average passenger per metro car' less than estimated, by a factor of 0.9340 which then equals to 292.9.

2) Carpool multiplier

In order to find the value of 'carpool multiplier', we refer to the average of occupants per vehicle entering central London during the morning peak over the years 2002 (before the implementation of the scheme) to 2006, found in London Travel Report (TFL, 2007b), Table 1.3.2 (p.6) which part of the table is shown in Table B.1:

Table B.1- Carpool Multiplier

People per Vehicle	1.36	1.35	1.37	1.39	1.38
year	2002	2003	2004	2005	2006

3) Average lifetime of metro cars

According to the history of London Underground rolling stock found on different websites (Squarewheels.org.uk, 2011; TFL, 2011a; Tubeprune, 2007), a summary of dates of the introduction, withdrawal and lifetime of each underground rolling stock is provided in Table B.2. The 'average lifetime of metro cars' is calculated based on the LUL Rolling Stock from 1956 to present and on average is equal to 42.5 years (≈15512.5 days).

Table B.2- Average Lifetime of metro cars

stock (type of train)	cars	Trains	introduced	withdrawn	lifetime of stock
1956(prototype)		3	1956	2000	44
1959		76	1959	2000	41
1960(prototype)	24	3	1960	1994	34
A60	248		1960	2013	53
A62	216		1962	2013	51
1962			1962	1999	37
1967	316	39.5	1967	2012	45
C69	212	35	1970	present	
1972	252	63	1972	present	
1973	528	88	1975	present	
C77	67	11	1977	present	
D78	450	75	1980	2015	35
1983		30	1984-1989	1998	
1986(prototype)	12	3	1986	1989	3
1992	700	95	1993	present	
1995	636	106	2001	present	
1996	441	63	1997	present	
2009	8 cars per train		2009	present	
S	1255	191	2010		
In service	**4066**			Present	Average Lifetime=42.5 Years

4) Time for order and Delay in receiving metro cars

Similarly, according to the history of the London Underground rolling stock found on different websites (Squarewheels.org.uk, 2011; Tubeprune, 2007) , the order date, first delivery and final delivery of some of the underground rolling stock is estimated as shown in Table B.3. So, 'time for order' and 'delay in receiving metro cars' is calculated based on the LUL (Not DLR Rolling Stock) which results into average values of 2.75 and 3 years respectively:

Table B.3- Time for Order and Delay in Receiving Metro Cars

Stock	ordered	first deliver	final deliver	Time for Order	Delay in Receiving Metro Cars
C	1968	1970		2	
D	1976	1980	1983	4	3
1983	1982	1984		2	
1995		1998	2001	3	3
2009		2009	2012		3
S		2010	2013		3
Average (Years)				2.75	3

5) Cost per metro car

With respect to the 'cost per metro car', the train web site (Tubeprune, 2007) describes that 30½ 8-car trains of the 1967 Tube Stock would cost £2.25 million in 1964, but today only 3 cars can be afforded with the same amount of money. In other words, if we divide £2.25 million by three, we find the parameter 'cost per metro car' at about £750000.

6) Discounts for local residents, fleet vehicle and disabled people and respective fractions

In the congestion pricing scheme implemented in London, some exemptions are considered for local residents, fleet vehicle and disabled people. According to the Impacts Monitoring-Third Annual Report (TFL, 2005), "…residents of the congestion charging zone can register for a 90 percent discount (for a minimum weekly payment), and disabled persons' Blue Badge holders and certain alternative fuel vehicles are eligible for a 100 percent discount" (p. 9). However, the data regarding the 'total car demand' in our model, is based on the Impacts Monitoring-Third Annual Report (TFL, 2005) that has been indicated by the term "traffic entering the central London charging zone during charging hours" and does not include local residents. So, we disregard discounts for local residents in our model.

However, the total car demand does not include local residents, because it quotes "traffic entering the central London charging zone during charging hours". Also, there is a certain type of charge considered for fleets of business vehicles. If vehicles are registered through a Fleet account, need to pay £5.5 pre-July 2005 which is 10% above the standard daily vehicle charge of £5 and have to pay £7 post-July 2005 which is 12.5% less than standard daily vehicle charge of £8 (TFL, 2006) (p. 174, table 9.3)[17].

17 So in order to include the discount /raise for fleet vehicle, a step function is used which adds 2.25% at beginning of July year 2005 (i.e. -0.1+STEP(0.225,942)).

In order to find ‘fraction of fleet vehicle’ parameter, we refer to the ‘Impacts Monitoring-Third Annual Report Final’ (TFL, 2005). In the report, it has been stated that “…of the payments, 16 percent are made in respect of vehicles registered for the 90 percent residents’ discount, 11 percent are made for fleet vehicles and 73 percent are made in respect of other vehicles” (p. 141). So, the ‘fraction of fleet vehicle’ and the ‘fraction of local resident’ parameters of the model are set to 0.11 and 0.16 respectively.

Therefore, ‘total cars subject to pricing’ is found by dividing ‘fraction of fleet vehicle’ by (1-fraction of local resident) so that the true fraction of non-resident car drivers who own fleet vehicle is found. Also we have to eliminate the fraction of disabled people or Blue-Badge from the total demand initially and then multiply by other fractions of discount. According to Table 8.3 on page 112 of Impacts Monitoring-Second Annual Report (TFL, 2004), 18000 are Residents of Zone which use daily discount. So this makes the total population 112,500 daily (18000/0.16), and then Blue-Badge or disabled people are 8000 over 112,500 people which finds the ‘fraction of disabled people’ parameter of the model as 0.071111.

7) Fraction implementation and the delay for spending on implementing the scheme

The total revenue accumulated is partially allocated for improving metro rail capacity based on metro demand. Also a small percentage is assigned for the pricing scheme implementation. The remainder is collected and not spent at all. In other words, we only consider spending part of the revenue on buying extra metro cars and save the rest in ‘total budget stock’ without spending on other operating costs such as paying administration and contractors or on any kind of other programs including contributions to increase bus frequency, research and analysis and accident remedial measures, reducing child accidents, walking and cycling and making distribution of goods into and around London more sustainable (TFL, 2005) (page 139, figure 94).

In order to find the percentage assigned for the implementation of the pricing scheme, which is termed ‘fraction implementation’ in the model, we refer to Federal Highway Administration report (FHWA, 2008) stating that, “the initial costs of setting up the Scheme was £161.7m” (p. 2-15). We assume that the amount is spent yearly and so the ‘appropriation delay for pricing scheme money’ is set to one year (i.e. 365 days). Also, if we divide this amount over the whole period of years 2003 to 2008 (i.e. 6 years), it would make about £32.34m per year and that is about 25.1549% of revenues per year until the end of year 2008 (i.e. time 1825) which defines the value of ‘fraction implementation’ parameter in the model. As described earlier, in our model we do not take into account any other kind of operating costs and just save the remainder of the accumulated revenue which has not been spent on buying extra metro cars.

8) Maximum acceptable congestion charge

The parameter 'maximum acceptable congestion charge' defines people's perception towards the congestion price. Since before implementing the pricing scheme, there was no charge in entering the central London area, by imposing such cost, it is reasonable to assume that the congestion charge is regarded as a *high* value in people's perception. So the maximum acceptable congestion charge should also be regarded the same value as the congestion charge. However, after some years, probably the maximum acceptable congestion charge might increase because drivers get used to paying the initial charging price. This is the reason that policy makers should consider increasing the charging cost in future which is also been considered in the London pricing scheme (i.e. the charging cost was increased in July 2005 to £8). This issue is further discussed in Section 6, sensitivity analysis of the paper.

9) Highway capacity

In order to determine the variable 'highway capacity' in the model, no data was found to assign a value for this parameter. So, instead we used the 'highway utilization' value, without impacting the underlying methodology. In our approach, 'highway utilization' is found by multiplying the 'maximum number of cars on roads' and 'maximum trip length'. For the 'maximum trip length' value, we consider the 'average trip miles' (mile/person/Day) that passengers traveled (per person per day) in Central London during weekdays, reported since 1991 (See Table 8), and choose the highest value which is in year 2001, equal to 12.3 kilometers (i.e. 7.64287 miles).

10) Maximum number of cars on roads

In order to determine the parameter 'maximum number of cars on roads', based on the fact that before the implementation of the pricing scheme in year 2003, London was very congested, so for the initial setting of the model, density on roads should be high and perceived density on roads should have the maximum *high* membership domain. So, we postulate the normalized density on roads should be about 1 initially. With the initial car demand of 515,200 passengers in year 2003, and the average carpool multiplier of 1.37 passenger/car, the value of 'maximum number of cars' should not exceed the number of cars driving on the highly congested roads back in year 2003 (i.e. 515,200 divided by 1.37) which is 376,059 cars. So, the value of the parameter 'maximum number of cars', is set equal to this upper bound (i.e. 376,059 cars).

Appendix C- Loop Knockout

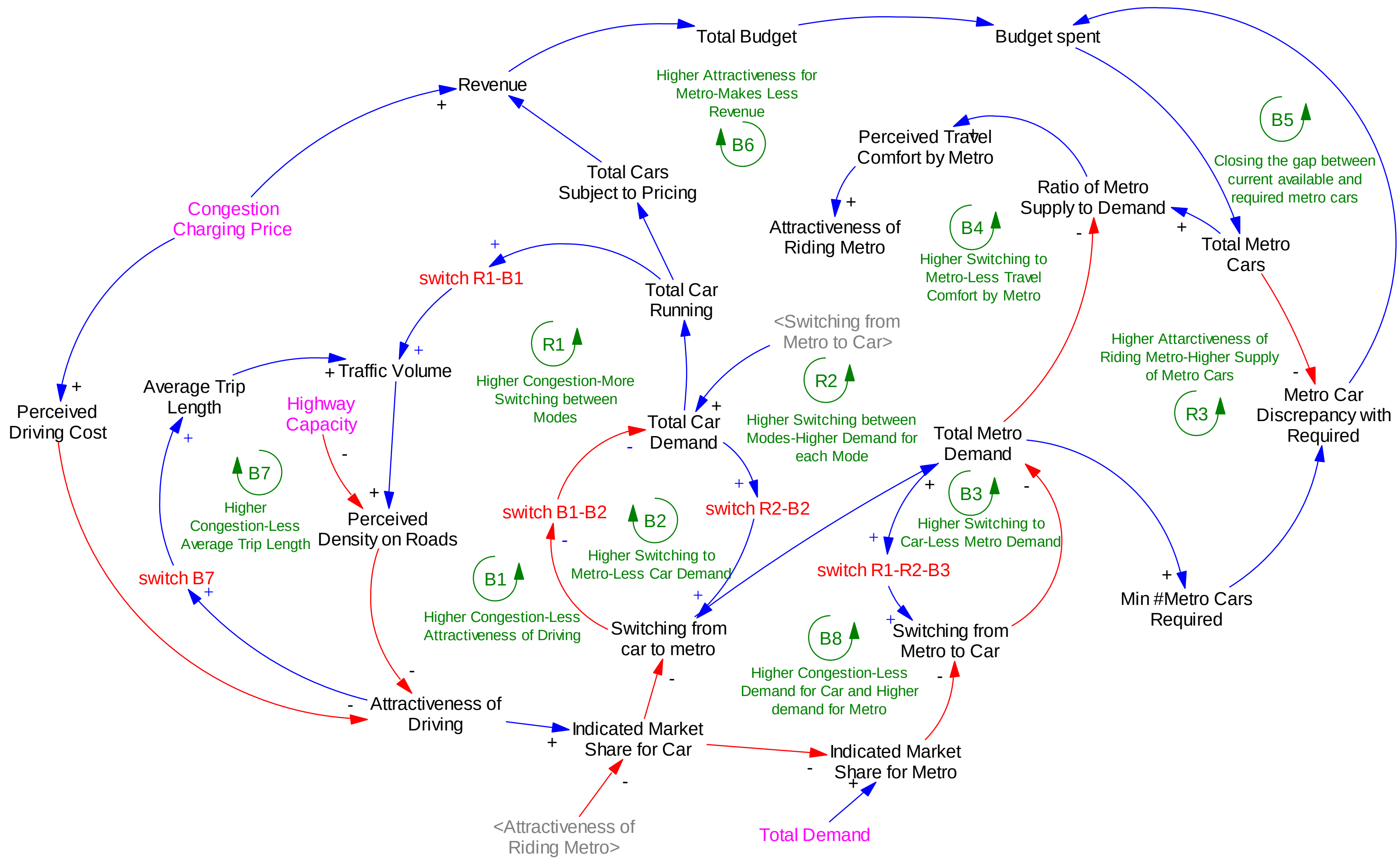

Figure C.1- The links shutdown for knocking out certain loops

The switch variables shown in Figure C.1 are coded as below:

test time=150
Units: day

switchB7=SAMPLE IF TRUE ((Time < test time), Attractiveness of Driving Car normalized, Attractiveness of Driving Car normalized)
Units: mile/trip

"switchR2-B2"=SAMPLE IF TRUE ((Time < test time), Total Car Demand, Total Car Demand)
Units: passenger

"switchR1-B1"=SAMPLE IF TRUE ((Time < test time), total car running, total car running)
Units: car

"switchR1-R2-B3"=SAMPLE IF TRUE ((Time < test time), Total Metro Demand, Total Metro Demand)
Units: passenger

"switchB1-B2"=SAMPLE IF TRUE ((Time < test time), switching from car to metro, switching from car to metro)
Units: passenger/day

Appendix D – The Code

Indicated Average Trip Length=Maximum trip length*POWER(Attractiveness of Driving Car normalized, Strength of Impact on Trip Length)

Units:mile

Min Metro Cars Required=Total Metro Demand/(average passenger per metro car)

Units:metro car

Initial Min Metro Cars Required=MD Value/(average passenger per metro car)

Units:metro car

change in trip length=(Indicated Average Trip Length-Average Trip Length)/Time to change trip length

Units:mile/day

Attractiveness of Riding Metro Normalized=MAX((Attractiveness of Riding Metro based on COA-0.1667), 0)/(0.833367-0.1667)

Units:Dmnl

Indicated Market Share for Car=Total Demand*((Attractiveness of Driving Car normalized)/((Attractiveness of Driving Car normalized)+(Attractiveness of Riding Metro Normalized)))

Units:passenger

Attractiveness of Driving Car normalized=MAX((Attractiveness of Driving Car Including Cost based on COA-0.388922) , 0)/(0.611144-0.388922)

Units:Dmnl

Normalized ratio of metro supply to demand=if then else (ratio of metro supply to demand<=1, ratio of metro supply to demand, 1)

Units:Dmnl

Attractiveness of Driving Car Including Cost based on COA=SUM(uL[D!]*x value[D!])/SUM(uL[D!])

Units:Dmnl

uL 0[D]=MAX(MIN(scm maxL, 1-2*x value[D]), MAX(MIN(scm maxM, MIN(2*x value[D], 2-2*x value[D])) , MIN(scm maxH, -1+2*x value[D])))

Units:Dmnl

uL[D]=MAX(MIN(max valueL, 1-2*x value[D]), MAX(MIN(max valueM, MIN(2*x value[D], 2-2*x value[D])) , MIN(max valueH, -1+2*x value[D])))

Units:Dmnl

Attractiveness of Riding Metro based on COA=SUM(uL 0[D!]*x value[D!])/SUM(uL 0[D!])

Units:Dmnl

x value[d1]=   0.0001

x value[d2]= 0.0002
x value[d3]= 0.0003
.
.
.
x value[d9999]=0.9999
x value[d10000]= 1
Units:Dmnl

Max Spending rate=Total Budget/Time for Order
Units:pound/day

Normalized ratio of work travel cost to trip budget=if then else (ratio of travel cost to work trip budget>=0.9, 1, ratio of travel cost to work trip budget)
Units:Dmnl

Highway Capacity=Maximum Number of Cars on Roads*Maximum trip length
Units:car*mile

Traffic Volume=total car running*Average Trip Length
Units:car*mile

total cars subject to pricing=total car running*(1-fraction of disable people)*(1-(fraction of fleet vehicle/(1-fraction of local resident))+fraction of fleet vehicle*(1-discount for fleet vehicle)/(1-fraction of local resident))
Units:car

total cars subject to pricing Initial=CD initial*(1-fraction of disable people)*(1-(fraction of fleet vehicle/(1-fraction of local resident))+fraction of fleet vehicle*(1-discount for fleet vehicle)/(1-fraction of local resident))/carpool multiplier
Units:car

funding used for metro=Revenue from Pricing Scheme/appropriation delay for Revenue
Units:pound/day

switching from metro to car=MAX((Total Metro Demand-Indicated Market Share for Metro), 0)/time with metro before switching
Units:passenger/day

scm maxH="fuzzy rule for switching c-m"[scmr3]
Units:Dmnl

scm maxL="fuzzy rule for switching c-m"[scmr1]
Units:Dmnl

scm maxM="fuzzy rule for switching c-m"[scmr2]
Units:Dmnl

Indicated Market Share for Metro=Total Demand-Indicated Market Share for Car
Units:passenger

Total Car Demand= INTEG (switching from metro to car-switching from car to metro,CD initial)
Units:passenger

Total Metro Demand= INTEG (switching from car to metro-switching from metro to car,MD Value)
Units:passenger

switching from car to metro=MAX((Total Car Demand-Indicated Market Share for Car), 0)/time with car before switching
Units:passenger/day

max valueM=(Fuzzy Rule Definition[r3]+(Fuzzy Rule Definition[r5]+Fuzzy Rule Definition[r7]))/3
Units:Dmnl

max valueH=(Fuzzy Rule Definition[r1]+(Fuzzy Rule Definition[r2]+Fuzzy Rule Definition[r4]))/3
Units:Dmnl

max valueL=(Fuzzy Rule Definition[r6]+(Fuzzy Rule Definition[r8]+Fuzzy Rule Definition[r9]))/3
Units:Dmnl

discount for fleet vehicle=-0.1+STEP(0.225,942)
Units:Dmnl

fraction of fleet vehicle=0.11
Units:Dmnl

"1/std 0"[variables]=ZIDZ(1, Std 0[variables])
Units:Dmnl

"1/std"[variables]=ZIDZ(1, Std[variables])
Units:Dmnl

"1/stdATL 0"="1/std 0"[v5]
Units:Dmnl

"1/stdATL"="1/std"[v5]
Units:Dmnl

"1/stdMetroCar 0"="1/std 0"[v3]
Units:Dmnl

"1/stdMetroCar"="1/std"[v3]
Units:Dmnl

"1/stdRevenue 0"="1/std 0"[v4]
Units:Dmnl

"1/stdRevenue"="1/std"[v4]
Units:Dmnl

"1/stdTCD 0"="1/std 0"[v2]
Units:Dmnl

"1/stdTCD"="1/std"[v2]
Units:Dmnl

"1/stdTMD 0"="1/std 0"[v1]
Units:Dmnl

"1/stdTMD"="1/std"[v1]
Units:Dmnl

M Y 0[variables]=ZIDZ(Sum of Yi 0[variables] ,Count[variables])
Units:Dmnl
~ Mean of y (sum y)/n

TotalMetroCarsdata
Units:metro car

Start Time[v1]= 0
Start Time[v2]= 0
Start Time[v3]= 0
Start Time[v4]= 638
Start Time[v5]= 0
Units:day
~ Date of first data point

Std[variables]=if then else(MY2[variables] >POWER((M Y[variables]), 2) , SQRT(MY2[variables] - POWER((M Y[variables]), 2)) , 0)
Units:Dmnl
~ Standard Deviation of y. Calculated using the 'hand computation' formula to calculate the standard deviation without prior knowledge of the mean. Sterman (1984), pg. 64

ATLerror=Average Trip Length-AverageTripLengthdata
Units:mile

wTCD0=weightTCD 0
Units:Dmnl

TCDdata
Units:passenger

```
"Sum of Past Y^2 0"[variables]= INTEG (POWER((Yi 0[variables]), 2 ) /dt[variables],0)
	Units:Dmnl
	~	Sum of y^2 for previous points.

AverageTripLengthdata
	Units:mile

Sum of Past Yi[variables]= INTEG (Yi[variables] /dt[variables],0)
	Units:Dmnl
	~	Sum of y's that precede the current value.

Sum of Past Yi 0[variables]= INTEG (Yi 0[variables] /dt[variables],0)
	Units:Dmnl
	~	Sum of y's that precede the current value.

"Sum of Y^2 0"[variables]="Sum of Past Y^2 0"[variables] +POWER((Yi 0[variables]), 2 )
	~	Dmnl
	~	Sum of y^2.
	|

"Sum of Y^2"[variables]="Sum of Past Y^2"[variables] +POWER((Yi[variables]), 2 )
	Units:Dmnl
	~	Sum of y^2.

Sum of Yi[variables] =Sum of Past Yi[variables] +Yi[variables]
	Units:Dmnl
	~	Sum of y's.

Sum of Yi 0[variables] =Sum of Past Yi 0[variables] +Yi 0[variables]
	Units:Dmnl
	~	Sum of y's.

weightATL 0=GET XLS CONSTANTS('calibrationWeights.xls', 'Traffic','B5')
	Units:Dmnl

weightMetroCars=GET XLS CONSTANTS('calibrationWeights.xls', 'Traffic','B3')
	Units:Dmnl

weightMetroCars 0=GET XLS CONSTANTS('calibrationWeights.xls', 'Traffic','B3')
	Units:Dmnl

Count[v1]=Count for Past Points[v1]+pick[v1]
Count[v2]=Count for Past Points[v2]+pick[v2]
Count[v3]=Count for Past Points[v3]+pick[v3]
Count[v4]=Count for Past Points[v4]+pick[v4]+1
Count[v5]=Count for Past Points[v5]+pick[v5]
```

```
            Units: Dmnl
            ~           Counter for # of points.

Count for Past Points[variables]= INTEG (
            pick[variables]/dt[variables],
                        0)
            Units: Dmnl
            ~           Counter for # of previous points.

weightTCD=GET XLS CONSTANTS('calibrationWeights.xls', 'Traffic','B2')
            Units: Dmnl

weightTCD 0=GET XLS CONSTANTS('calibrationWeights.xls', 'Traffic','B2')
            Units: Dmnl

weightTMD=GET XLS CONSTANTS('calibrationWeights.xls', 'Traffic','B1')
            Units: Dmnl

weightTMD 0=
            GET XLS CONSTANTS('calibrationWeights.xls', 'Traffic','B1')
            Units: Dmnl

MY2[variables]=ZIDZ("Sum of Y^2"[variables] ,Count[variables])
            Units: Dmnl
            ~           Mean of y^2 (sum y^2)/n

dt[variables]=TIME STEP
            ~           day

wRevenue=weightRevenue
            Units: Dmnl

Final Times[v1]=1460
Final Times[v2]=1460
Final Times[v3]=2920
Final Times[v4]=1733
Final Times[v5]=2190
            Units: day

wTCD=weightTCD
            Units: Dmnl

Yi[variables]=Y[variables]*pick[variables]
            Units: Dmnl
            ~           Sampled simulated variable

one pound=1
```

Units: pound

TCDerror=Total Car Demand-TCDdata
Units: passenger

one mile=1
Units: mile

one passenger= 1
Units: passenger
~ In order to match the units

Y 0[v1]=TMDdata/one passenger
Y 0[v2]=TCDdata/one passenger
Y 0[v3]=TotalMetroCarsdata/one metro car
Y 0[v4]=Revenuedata/one pound
Y 0[v5]=AverageTripLengthdata/one mile
Units: Dmnl
~ The simulated data series

M Y[variables]= ZIDZ(Sum of Yi[variables] ,Count[variables])
Units: Dmnl
~ Mean of y (sum y)/n

Yi 0[variables]=Y 0[variables]*pick[variables]
Units: Dmnl
~ Sampled simulated variable

TMCerror=Total Metro Cars-TotalMetroCarsdata
Units: metro car

TMDdata
Units: passenger

TMDerror=Total Metro Demand-TMDdata
Units: passenger

Std 0[variables]=if then else(MY2 0[variables] >POWER((M Y 0[variables]), 2), SQRT(MY2 0[variables] - POWER((M Y 0[variables]), 2)) , 0)
Units: Dmnl
~ Standard Deviation of y. Calculated using the 'hand computation' formula to calculate the standard deviation without prior knowledge of the mean. Sterman (1984), pg. 64

variables: (v1-v5)

weightRevenue=GET XLS CONSTANTS('calibrationWeights.xls', 'Traffic','B4')
Units: Dmnl

weightRevenue 0=GET XLS CONSTANTS('calibrationWeights.xls', 'Traffic','B4')
Units: Dmnl

"Sum of Past Y^2"[variables]= INTEG (POWER((Yi[variables]), 2)/dt[variables], 0)
Units: Dmnl
~ Sum of y^2 for previous points.

Revenuedata
~ pound

Interval[v1]=365
Interval[v2]=365
Interval[v3]=365
Interval[v4]=365
Interval[v5]=365
Units: day
~ Interval between data points

weightATL=GET XLS CONSTANTS('calibrationWeights.xls', 'Traffic','B5')
Units: Dmnl

wMetroCars=weightMetroCars
Units: Dmnl

MY2 0[variables]=ZIDZ("Sum of Y^2 0"[variables] ,Count[variables])
Units: Dmnl
~ Mean of y^2 (sum y^2)/n

wRevenue0=weightRevenue 0
Units: Dmnl

RevenueError=Revenue from Pricing Scheme-Revenuedata
Units: pound

wTMD= weightTMD
Units: Dmnl

one metro car= 1
Units: metro car

Y[v1]=TMDerror/one passenger
Y[v2]=TCDerror/one passenger
Y[v3]=TMCerror/one metro car
Y[v4]=RevenueError/one pound
Y[v5]=ATLerror/one mile
Units: Dmnl

~ The simulated data series

wATL0=weightATL 0
Units: Dmnl

wATL=weightATL
Units: Dmnl

wTMD0=weightTMD 0
Units: Dmnl

pick[v1]=STEP(1,Start Time[v1])*(1-STEP(1,Final Times[v1] + TIME STEP/2))*if then else(Time/Interval[v1]= INTEGER(Time/Interval[v1]),1 , 0)
pick[v2]=STEP(1,Start Time[v2])*(1-STEP(1,Final Times[v2] + TIME STEP/2))*if then else(Time/Interval[v2]= INTEGER(Time/Interval[v2]),1 , 0)
pick[v3]=STEP(1,Start Time[v3])*(1-STEP(1,Final Times[v3] + TIME STEP/2))*if then else(Time/Interval[v3]= INTEGER(Time/Interval[v3]),1 , 0)
pick[v4]=STEP(1,Start Time[v4])*(1-STEP(1,Final Times[v4] + TIME STEP/2))*if then else((Time-Start Time[v4])/Interval[v4]= INTEGER((Time-Start Time[v4])/Interval[v4]),1 , 0)
pick[v5]=STEP(1,Start Time[v5])*(1-STEP(1,Final Times[v5] + TIME STEP/2))*if then else(Time/Interval[v5]= INTEGER(Time/Interval[v5]),1 , 0)
Units: Dimensionless
~ Takes a value of one for every data point available, assuming the data are \
available at intervals of Interval between the Start Time and End Time.

wMetroCars0=weightMetroCars 0
Units: Dmnl

Strength of Impact on Trip Length=0.0106844
Units: Dmnl

Fuzzy Rule Definition[r1]=(Perceived Density on Roads[FLow] +Perceived Driving Cost[TVCLow])/2
Fuzzy Rule Definition[r2]=(Perceived Density on Roads[FLow] +Perceived Driving Cost[TVCMedium])/2
Fuzzy Rule Definition[r3]=(Perceived Density on Roads[FLow] +Perceived Driving Cost[TVCHigh])/2
Fuzzy Rule Definition[r4]=(Perceived Density on Roads[FMedium]+ Perceived Driving Cost[TVCLow])/2
Fuzzy Rule Definition[r5]=(Perceived Density on Roads[FMedium] +Perceived Driving Cost[TVCMedium])/2
Fuzzy Rule Definition[r6]=(Perceived Density on Roads[FMedium] +Perceived Driving Cost[TVCHigh])/2
Fuzzy Rule Definition[r7]=(Perceived Density on Roads[FHigh] +Perceived Driving Cost[TVCLow])/2
Fuzzy Rule Definition[r8]=(Perceived Density on Roads[FHigh] +Perceived Driving Cost[TVCMedium])/2
Fuzzy Rule Definition[r9]=(Perceived Density on Roads[FHigh]+Perceived Driving Cost[TVCHigh])/2
Units: Dmnl

Average Trip Length= INTEG (change in trip length,Maximum trip length*POWER(1, Strength of Impact on Trip Length))
Units: mile

ratio of travel cost to work trip budget=congestion charging price/Maximum Acceptable Congestion Charge

Units: Dmnl

Maximum trip length=7.64287

Units: mile

~ This is the equivalent mileage (i.e. 12.3 km) that passengers traveled (per person per day) in year 2001 in Central London during weekdays which is considered the maximum trip length when attractiveness of driving car is at maximum value and equal to 1.

Time to change trip length=872.626

Units: day

Maximum Number of Cars on Roads=376058

Units: car

Maximum Acceptable Congestion Charge=5

Units: pound/(car*day)

Total Demand= INITIAL(CD initial+MD Value)

Units: passenger

congestion charging price=5+STEP(3,942)

Units: pound/(car*day)

~ This is the congestion charging price enforced in year 2003 by implementing the congestion pricing scheme.

passenger by metro per charging period=Total Metro Cars*average passenger per metro car

Units: passenger

Revenue from Pricing Scheme= INTEG (revenue accumulation-funding used for metro-funding used for pricing scheme implementation ,0)

Units: pound

~ congestion charging price*total cars subject to pricing Initial/funding factor

revenue accumulation= congestion charging price*total cars subject to pricing

Units: pound/day

ratio of metro supply to demand=XIDZ(passenger by metro per charging period , Total Metro Demand , 1)/0.934

Units: Dmnl

total car running=Total Car Demand/carpool multiplier

Units: car

MD Value=1.275e+006

Units: passenger

Money Required for MetroCars Shortage=cost per metro car*metro car discrepancy with allowable and required

Units: pound

Money Required for Replacement=cost per metro car*metro car aging*Time for Order

Units: pound

Money Allocated for purchasing Metro Cars=MIN(Desired Spending Rate, Max Spending rate)

Units: pound/day

Desired Spending Rate= Desired Money for Order/Time for Order

Units: pound/day

Min Time Required for Spending=1003.75

Units: day

metro car aging=Total Metro Cars/ metro car life time

Units: metro car/day

Desired Money for Order=Money Required for MetroCars Shortage+Money Required for Replacement

Units: pound

money spent for metro cars=(Budget Allocated for Buying Metro Cars)/(Delay in Receiving Metro Cars)

Units: pound/day

metro car discrepancy with allowable and required=MAX(MIN("allowable metro capacity within cordon-based area" , Min Metro Cars Required)-(Total Metro Cars+Metro Cars Ordered), 0)

Units: metro car

Metro Cars Ordered=Budget Allocated for Buying Metro Cars/cost per metro car

Units: metro car

Delay in Receiving Metro Cars=1095

Units: day

Total Metro Cars= INTEG (metro car increment-metro car aging, MIN("allowable metro capacity within cordon-based area", Initial Min Metro Cars Required*(metro car life time/(metro car life time+ Delay in Receiving Metro Cars))))

Units: metro car

metro car increment=(money spent for metro cars)/(cost per metro car)

Units: metro car/day

Budget Allocated for Buying Metro Cars= INTEG (Money Allocated for purchasing Metro Cars-money spent for metro cars, Initial Min Metro Cars Required*cost per metro car*Delay in Receiving Metro Cars/(metro car life time+Delay in Receiving Metro Cars))

Units: pound

funding factor=(fraction implementation/appropriation delay for pricing scheme money)+(1/appropriation delay for Revenue)
Units: 1/day

appropriation delay for Revenue=30
Units: day
~ The delay in budget allocation to improving the metro system.

Total Budget= INTEG (funding used for metro -Money Allocated for purchasing Metro Cars,(congestion charging price*total cars subject to pricing Initial/(funding factor*appropriation delay for Revenue))* Min Time Required for Spending)
Units: pound

D:(d1-d10000)

fraction implementation=0.251549-STEP(0.251549, 1825)
Units: Dmnl

funding used for pricing scheme implementation=fraction implementation*Revenue from Pricing Scheme/appropriation delay for pricing scheme money
Units: pound/day

CD initial= INITIAL(515200)
Units: passenger

"fuzzy rule for switching c-m"[scmr1]=Perceived Travel Comfort by Metro[MLow]
"fuzzy rule for switching c-m"[scmr2]=Perceived Travel Comfort by Metro[MMedium]
"fuzzy rule for switching c-m"[scmr3]=Perceived Travel Comfort by Metro[MHigh]
Units: Dmnl

Perceived Travel Comfort by Metro[MLow]=if then else (Normalized ratio of metro supply to demand=0, 1, if then else (Normalized ratio of metro supply to demand>=0 :AND: Normalized ratio of metro supply to demand<=0.5, (0.5-Normalized ratio of metro supply to demand)/0.5, 0))
Perceived Travel Comfort by Metro[MMedium]=if then else (Normalized ratio of metro supply to demand>=0 :AND:Normalized ratio of metro supply to demand<=0.5, Normalized ratio of metro supply to demand/0.5, if then else (Normalized ratio of metro supply to demand>=0.5 :AND: Normalized ratio of metro supply to demand<=1, (1-Normalized ratio of metro supply to demand)/0.5, 0))
Perceived Travel Comfort by Metro[MHigh]=if then else (Normalized ratio of metro supply to demand>=0.5 :AND:Normalized ratio of metro supply to demand<=1, (Normalized ratio of metro supply to demand-0.5)/0.5, if then else (Normalized ratio of metro supply to demand>=1, 1, 0))
Units: Dmnl

Perceived Density on Roads [FLow]=if then else (Normalized Density on Roads=0, 1, if then else (Normalized Density on Roads>=0 :AND: Normalized Density on Roads<=0.5, (0.5-Normalized Density on Roads)/0.5, 0))

Perceived Density on Roads[FMedium]= if then else (Normalized Density on Roads>=0:AND:Normalized Density on Roads<=0.5, Normalized Density on Roads/0.5, if then else (Normalized Density on Roads>=0.5 :AND:Normalized Density on Roads<=1, (1-Normalized Density on Roads)/0.5, 0))
Perceived Density on Roads[FHigh]=if then else (Normalized Density on Roads>=0.5:AND:Normalized Density on Roads<=1, (Normalized Density on Roads-0.5)/0.5, if then else (Normalized Density on Roads>=1, 1, 0))

Units: Dmnl

Perceived Driving Cost[TVCMedium]=if then else (Normalized ratio of work travel cost to trip budget>=0 :AND: Normalized ratio of work travel cost to trip budget <=0.5, Normalized ratio of work travel cost to trip budget/0.5, if then else (Normalized ratio of work travel cost to trip budget >=0.5 :AND: Normalized ratio of work travel cost to trip budget<=1, (1-Normalized ratio of work travel cost to trip budget)/0.5, 0))
Perceived Driving Cost[TVCLow]=if then else (Normalized ratio of work travel cost to trip budget=0, 1, if then else (Normalized ratio of work travel cost to trip budget >=0 :AND: Normalized ratio of work travel cost to trip budget<=0.5, (0.5-Normalized ratio of work travel cost to trip budget)/0.5, 0))
Perceived Driving Cost[TVCHigh]=if then else (Normalized ratio of work travel cost to trip budget>=0.5 :AND: Normalized ratio of work travel cost to trip budget <=1, (Normalized ratio of work travel cost to trip budget-0.5)/0.5, if then else (Normalized ratio of work travel cost to trip budget >=1, 1, 0))

Units: Dmnl

time with car before switching= 2987.82

Units: day

switching car to metro: scmr1, scmr2, scmr3

Units: Dmnl

Normalized Density on Roads=MIN(1, Traffic Volume/Highway Capacity)

Units: Dmnl

Range:(r1-r9)

Flow Rate:FLow, FMedium, FHigh

Units: Dmnl

Trip Value and Cost: TVCLow, TVCMedium, TVCHigh

Units: Dmnl

Metro S and D: MLow, MMedium, MHigh

Units: Dmnl

average passenger per metro car=292.88

Units: passenger/metro car

~ This is the average number of passengers riding metro during the charging \
hours in a day. It is based on data from London Cordon Area.

time with metro before switching=720

Units: day

"allowable metro capacity within cordon-based area"=8000
Units: metro car
~ This is the maximum allowable metro capacity within the cordon-based area. However, since there is no data for this parameter, we assume that it is a high value so that it does not shut down the loop of increasing the number of metro cars for the London Cordon area.

carpool multiplier=1.37
Units: passenger/car

metro car life time=15512.5
Units: day

cost per metro car=750000
Units: pound/metro car

Time for Order=1003.75
Units: day

appropriation delay for pricing scheme money=365
Units: day
~ The delay in budget allocation to implementing the pricing scheme.

fraction of local resident=0.16
Units: Dmnl

fraction of disable people=0.07
Units: Dmnl

****
The Following are Simulation Control Parameters
***~

FINAL TIME = 7200
Units: day
~ The final time for the simulation.

INITIAL TIME = 0
Units: day
~ The initial time for the simulation.

SAVEPER = TIME STEP
Units: day [0,?]
~ The frequency with which output is stored.

TIME STEP = 1
Units: day [0,?] ~ The time step for the simulation.

Third Essay:

Basal Metabolic Rate: Systematic Review and Meta-Regression for Proposing General Prediction Equations

Abstract

Basal Metabolic Rate is the largest component of total energy expenditure and thus a major contributor to energy balance. Current literature includes several equation structures that have been estimated in multiple different studies for predicting Basal Metabolic Rate for different demographic groups. We conduct a comprehensive literature search and compile 248 studies that estimate Basal Metabolic Rate (or closely related measures) based on macro independent variables (Age, Gender, Ethnicity, Fat-Free Mass, Fat Mass, Height, Waist-to-Hip Ratio, Body Mass Index, and Weight). A subset of 47 studies includes enough details to allow us to combine similarly structured equations for similar population groups and develop meta-regression equations. We develop meta-equations for 20 different population groups, using different subsets of 17 equation structures found in the literature. This review therefore provides a comprehensive summary of what equation forms are available for predicting Basal Metabolic Rate for different subpopulations, and how reliable they are. The review can assist practitioners and researchers in finding the best-suited equations, depending on data availability and the purpose of a project.

Key Words and Phrases: Basal Metabolic Rate, Resting Metabolic rate, Prediction, Meta-Analysis, Review, Meta-Regression

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1. Introduction

During the past four decades, there has been an alarming increase in obesity in the U.S. and many other countries. The percentage of Americans who are obese has doubled to nearly 30%, and close to two-thirds of the population is overweight (Bray & Bouchard, 2004; Ogden et al., 2006). Models that can assess the potential impact of alternative interventions at the individual and societal levels are much needed for turning around the obesity trend. Rahmandad and Sabounchi (2011) study the dynamics of obesity in the United States over time to build a generic system dynamics model that can be used for obesity policy analysis at multiple levels. The model builds on individual-level energy models of Hall (2010) and Butte, Christiansen, & Sorensen (2007) to capture the energy balance and weight change throughout the life of individuals, and aggregates individual-level models to population-level trends. The model takes physical activity and energy intake as inputs and provides the dynamics of body weight and body composition as outputs. The model is calibrated against National Health and Nutrition Examination Survey (NHANES) data. The calibration simultaneously fits body weight model outputs against the same distributions in data for 110 population subgroups. However, the simulation results do not fit the NHANES data as closely as desired. One reason is that current dynamic energy balance models do not consider the dependence of Basal Metabolic Rate (BMR) on age, ethnicity, and gender. Since BMR constitutes a significant portion of total energy expenditure of the body, this problem can lead to general biases in the population-level model (Rahmandad & Sabounchi, 2011).

The Basal Metabolic Rate, defined as the energy required for performing vital body functions while the body is at rest, contributes to 60-75% of the total energy expenditure of the body (Abdel-Hamid, 2002; Poehlman, 1992). There are many statistical studies that have included age as an independent variable in explaining BMR (Cunningham, 1980; Cunningham, 1991; Harris & Benedict, 1919; Maffeis, Schutz, Micciolo, Zoccante, & Pinelli, 1993; Poehlman, 1992; John R. Speakman & Klaas R. Westerterp, 2010; Andrew M. Tershakovec, Kerri M. Kuppler, Babette Zemel, & Virginia A. Stallings, 2002; Vaughan, Zurlo, & Ravussin, 1991). Furthermore, several other studies find that BMR depends on the body composition (i.e., Fat Mass and Fat-Free Mass) (Cunningham, 1991) and/or gender and ethnicity (Bhopal & Rafnsson, 2009). The purpose of this study is to perform an extensive systematic review of studies exploring the relationship between BMR and different factors including age, body composition, gender, and ethnicity. These factors influencing BMR are studied so that BMR can also be included as an endogenous variable in the model of predicting body weight dynamics.

This study can potentially lead to more robust policy intervention in order to mitigate the increase in obesity, because underlying mechanisms that influence obesity have practical implications for intervention policies. For example, some in the literature argue that higher prevalence of obesity and difficulty in weight management derives from lower BMR (Ferraro et al., 1992; Andrew M. Tershakovec, et al., 2002) as people with low BMR are more susceptible to gaining weight. Others disagree; for example, Bogardus et al. (1986) find that subjects from families with a lower BMR (adjusted for FFM, Age and Sex), are no more obese than subjects from families with a higher BMR. They mention that when BMR is adjusted for FFM, then it is already adjusted for obesity, because FM and FFM are closely correlated. Ravussin and Rising, (1992) note that different opinions exist in the literature regarding differences between obese and lean subjects and their energy efficiency. These authors (1992) also mention that some literature argues that the obese may be more energy-efficient, meaning that they require fewer calories per unit of metabolic active tissue, and that some other literature states that overweight subjects have higher metabolic rates. Also, there are inconsistencies in how differences between metabolic rates of obese and lean subjects are reported, due to the methods by which metabolic rates are normalized. Some divide the total metabolic rates by FFM, but do not consider the fact that the linear relationship between BMR and FFM has a non-zero intercept (E Ravussin & Bogardus, 1989). Furthermore, the number of subjects used for each study is limited and may not truly represent the whole population. All these factors underline the importance of bringing together the results of different studies to estimate more reliable equations of how BMR depends on its various determinants.

1.1. Various Definitions of Basal Metabolic Rate

Total Energy Expenditure consists of three components, including Basal Metabolic Rate (BMR), physical activity and energy expended on thermogenesis induced by food intake, drugs, exposure to cold and other stress factors (Klausen, Toubro, & Astrup, 1997). Basal Metabolic Rate constitutes about 60-75% of the Total Daily Energy Expenditure and serves as the maintenance energy required for the basic homeostasis of the body (Abdel-Hamid, 2002; Poehlman, 1992). For individuals who have a sedentary lifestyle, BMR constitutes about 70% of their daily total energy expenditure (M. J. Muller & Bosy-Westphal, 2003).

While some have used Basal Metabolic Rate (BMR) and Resting Metabolic Rate (RMR) interchangeably (Bogardus, et al., 1986), others differentiate between the two based on the conditions under which they are measured. For example, Torun et al. (1996)(pS46) describe that "measurement conditions for quasi-basal is supine position, 10-12 h[ours] fasting, transported by vehicle to the laboratory, resting 30-60 min prior to measurement" (p. S46). Similarly, Sherman (1946) (p156) states that "basal metabolism is used to designate the energy metabolism of the body when at complete rest (both mentally and physically) in the so-called "post-absorptive state" (12 to 18 hours after the last intake of food) in a room of comfortable temperature and when the body temperature is within normal range."

In contrast, for RMR, the measurements are done in "supine, sitting and standing positions, 2-4 h after a light meal and resting for 15-45 min before the test" (Torun, et al., 1996) (pS46). Furthermore, they specify that "measurements of RMR should be between 15 and 20% higher than BMR, considering the conditions under which RMR is measured" (Torun, et al., 1996)(pS46).

In summary, we focus on studies that have measured Basal Metabolic Rate, based on the above conditions, that is in the post-absorptive state (i.e., at least after 10-12 h fasting). We note that these studies may have used other terms such as Resting Metabolic Rate (RMR), Resting Energy Expenditure (REE) or Basal Energy Expenditure (BEE) to capture the same concept.

1.2. Predicting Basal Metabolic Rate

Measurement of Basal Metabolic Rate is done through direct or indirect calorimetry (Ferrannini, 1988) which is costly and cumbersome, especially for children, infants and elderly; therefore, several different prediction equations have been evaluated in the literature to relax the need for direct measurement.

With regards to major determinants of Basal Energy Expenditure, different models exist in the literature. Muller and Westphal (2003) (p520) report that the estimates of energy requirements are conceptually representing group means and not individuals, and that usually predictive equations are based on measurements of several individuals. Age is one of the factors that influences BMR. Poehlman (Poehlman, 1992)(p2057) finds that "total daily energy expenditure and its components decline with advancing age." However, Speakman and Westerterp (2010) find that in older ages (>57.8 for men and >39.8 for Women), BMR is negatively related to age, whereas in the earlier years it is positively related to age. Furthermore, Roza and Shizgal (1984) explore BMR in adults 17 to 88 years of age, and state that if BMR is predicted from age and Body Cell Mass (BCM) (i.e., Total mass of metabolically active cells, i.e., the component of body composition which is responsible for all the oxygen consumption, CO_2 production and the work performed by the body), then BMR does not change with advancing age when BCM is constant.

Muller and Westphal (2003) (p519) claim that "Body Cell Mass, a familial trait, and thyroid status" are the significant terms in describing BMR. Muller et al. (2001) find, in patients with obesity class II and III, that the equation of Harris and Benedict (1919) predicted the average BMR with acceptable precision for clinical use and was better fitting than most of the currently available predictive equations for BMR. However, the recalculated version by Roza and Shizgal (1984) was more accurate and should therefore be used instead of the original equation. Also, the Harris and Benedict (1919) equation had sufficient precision in extremely obese subjects with a body weight >= 120 kg, so Muller et al. (2001) find no need for adaptation.

Lazzer et al. (2004) investigate the relationship between BMR and Fat-Free Mass (FFM) for obese adolescents who follow a weight reduction program. After significant weight loss, the BMR was still 6-12% lower after adjustment for FFM. The authors argue that, since BMR can also be estimated from tissue/organ masses and their corresponding metabolic rates, the unexpected differences of BMR values regarding FFM factor are related to significant decrease of metabolic rates of tissue/organ masses and also slower protein turnover due to less food intake. This implies that calculating BMR based on tissue/organ mass and metabolic rates is an appropriate method.

Most literature finds no difference between the BMRs of lean and obese adult subjects (Nelson, Weinsier, Long, & Schutz, 1992) or those of children (Molnar & Schutz, 1997). However, Muller et al. (2004) find significant differences in BMR between 5 to 91 years subjects of underweight, normal-weight, overweight and obese women and between obese men and other BMI groups, and Rodriguez et al. (2002) find different regressions for lean and obese children and adolescents.

Frankenfield et al. (2005) perform a systematic review and compare the four most commonly used BMR prediction equations in clinical practice – Mifflin et al. (1990), Owen (Owen et al., 1987; Owen et al., 1986), Harris and Benedict (1919), and WHO (1985) – in terms of reliability and accuracy for adults. They find that Mifflin et al. (1990) predicts BMR within 10% of measured BMR values in more obese and non-obese individuals, and also has the narrowest error range and hence is the most reliable among the four. For underrepresented groups of validation studies (older subjects and US-residing ethnic minorities including Black, Asian or Pacific Islander, American Indian, Alaskan Native or Hispanic populations), caution should be employed. In another review, Froehle (2008) has used group means as individual data, either by weighting the means by their sample size or just treating them as individual data, and then has run regressions over the dataset.

Based on this overview of the literature, there are several equations that estimate the BMR, using the same or different structural forms, for different demographic groups. These equations use different independent variables and come to somewhat inconsistent conclusions in a few cases. Therefore, picking a single equation for application in the dynamic modeling context that motivated this study was complicated. This fact induced us to perform a systematic review and conduct a meta-regression analysis to find the most appropriate model for predicting Basal Metabolic Rate for different subpopulations and demographic groups.

2. Overview of the systematic literature review and selection process

As Wang et al. (2000) describe, the models in the literature that predict Basal Metabolic Rate (BMR) include different determinants and metabolically active components at four different levels: molecular (Fat Mass and Fat-Free Mass), cellular (extracellular fluid and extracellular solids), tissue/organ, and whole body (Body Mass). In this Systematic Review, our purpose is to find all regression equations created in the literature for predicting Basal Metabolic Rate based on molecular or whole body-level factors. More detailed levels (cellular or tissue/organ) are not considered due to the complexity involved in quantifying those factors, which negates the value of BMR prediction equations (instead of direct measurement). In our review, the selected papers contain prediction models for healthy obese or non-obese individuals, differentiated based on their ethnicity, sex, and age. Then we apply a meta-regression analysis to generate a combined equation/model that is more robust in predicting BMR for each subpopulation group. In our study we refer to meta-regression analysis as a method to develop a single regression equation that summarizes the findings of multiple regressions found in a number of studies.

The comprehensive search of the literature is performed in four stages to identify all studies that predict a basal metabolic rate equation based on a dataset collected by the authors or adopted from another source. The specific keywords used to search PubMed and the Web of Science databases for studies published in any language between the earliest available date (October 31, 1923) and the latest (March 3, 2011) are shown in Figure 45. Any kind of publication which includes a prediction model for Basal Metabolic Rate (BMR) was selected. As described earlier, since BMR is also referred to in the literature as Resting Metabolic Rate (RMR), Resting Energy Expenditure (REE) or Basal Energy Expenditure (BEE), and often just the abbreviations such as BMR, RMR, and BEE are used, we included all these terms in our set of keywords. The resulting search leads to a broad range of items, including many non-relevant topics such as 'honey-BEE' or 'Rare-Earth-Elements (REEs)'. All of the titles/abstracts of 9787 papers/studies were reviewed in the first step to filter out the clearly unrelated papers.

In step 2, studies were excluded which, for example, focused on BMR of patients with disease or using any kind of drug/treatment, other compartments of energy expenditure or energy intake, and non-human BMR. The full set of exclusion criteria is shown in step 2 of Figure 45. Later, in step 3, by reviewing the full text of 970 remaining studies, 712 studies were excluded in this step due to the aforementioned criteria and some additional criteria including those which report a review or study the validity of existing BMR prediction methods/models, report comparison of BMR between different groups, focus on inter/intra-individual variance of BMR, studies without reporting the BMR prediction equation or just describing correlation values between BMR and different factors, focus on sleeping metabolic rate or postprandial BMR (not post-absorptive state, meaning after at least 10-12 hours fasting) and also some small percentage that were reported as retracted studies. Furthermore, 46 studies were excluded because they find the relation between BMR and factors at a cellular level, such as blood adipocytokines, pulse pressure and protein turnover. After this screening process, 248 studies which generate a model/regression for predicting BMR based on a data set of healthy obese or non-obese individuals were reviewed and coded. The details are described in the next section.

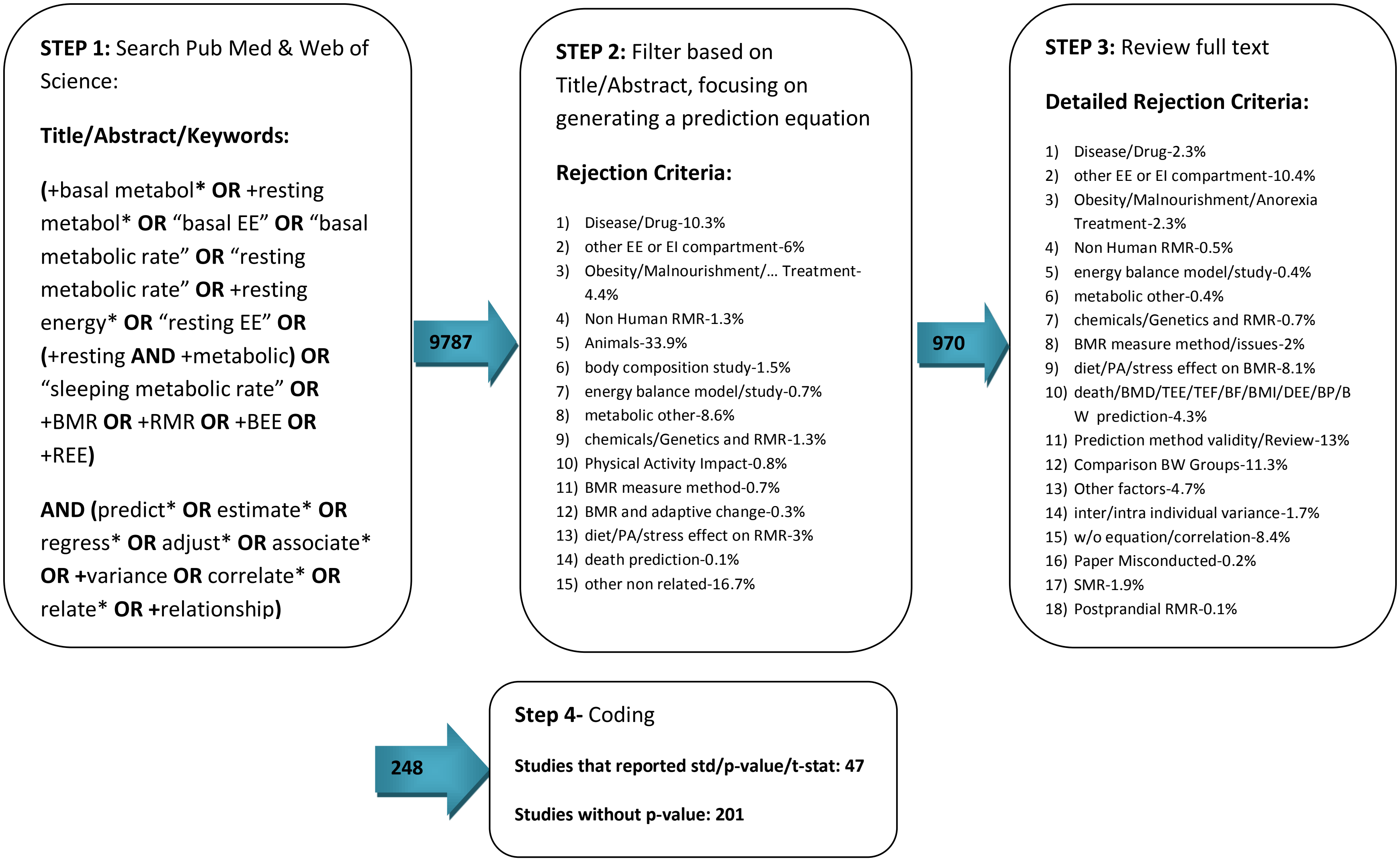

Figure 45 - Flowchart of literature search and selection process

3. The Coding Procedure

The final set of 248 papers is categorized into two groups. The first group, including 201 studies, are coded (for future research) by including the data sample size and determinants used to estimate BMR, but are not further analyzed in this paper because they lacked enough specificity to allow parametric meta-regression. The second group includes 47 studies that reported the standard deviation of the regression coefficients or a related statistic such as t-stat and p-value to estimate the standard deviation value. These studies allow meta-regression analysis and are included in the results reported in this paper. This category was coded by recording details of the data set used in the study and the equations developed (see Appendix A). Variance or standard deviation of reported regression parameters is needed for conducting meta-regression analysis. Therefore we follow a set of procedures (described in Appendix B) to consistently extract or estimate this factor.

4. Meta-Regression Results

There are different approaches in the literature for synthesizing slopes of a set of similar regressions found in different studies (Becker & Wu, 2007), which we refer to as meta-regression[18]. Some of these approaches, such as the multivariate Generalized Linear Square approach suggested by Becker and Wu (2007), draw on the correlations between different slopes and require using the covariance matrices of the regression slopes in synthesizing an average slope. This could potentially provide a robust estimate, but the covariance matrices are rarely reported in studies. In fact, none of the studies found in the literature search of this paper included the covariance matrices of slopes. A Weighted Least Squares (Univariate) approach used by Bini et al (2001) and applied in different studies (Manning et al., 2011; Ros, Temminghoff, & Hoffland, 2011) requires only having the regression coefficients and the standard error for each coefficient, which are usually reported by authors when running regressions. Then a weighted least square method can be applied to find a weighted average of the regression coefficients based on the following formula. Where k is the number of slopes combined, b_{ij} is the slope for factor x_j from study i and w_{ij} is the weight for that slope in the i[th] study calculated as follows:

$$b_{.j} = \frac{\sum_{i=1}^{k} w_{ij} b_{ij}}{\sum_{i=1}^{k} w_{ij}} \tag{1}$$

[18] In some literature, meta-regression is referred to as running a regression by considering a common summary statistic drawn from the primary studies as the dependent variable. In this method, the independent variables in the meta-regression include characteristics of the primary data, such as study design, valuation method, sample size, model specification, econometric methods, and other “quality” variables (J. Nelson & Kennedy, 2009).

$$w_{ij} = {}^{1}\!\big/_{Var(b_{ij})} \quad (2)$$

$$Var(b_{.j}) = {}^{1}\!\big/_{\sum_{i=1}^{k} w_{ij}} \quad (3)$$

Given the simplicity and feasibility of this approach, it is used to conduct meta-regression for the models found in this review. The systematic review has narrowed down the final set to forty-seven papers which report regression models for Basal Metabolic Rate (BMR) as the independent variable and the sets of determinants, with their corresponding standard deviation of each coefficient or a similar statistic such as the p-value or t-statistic that can be used to find an approximation of the standard deviation of the coefficients. The final set of studies is categorized into different groups based on the functional form of the regression and the determinants used in each. As a result, seventeen categories of Regression Models are identified. The structure of all these meta-regression structures is shown in Table 14 and their corresponding reference numbers are shown in each cell for every subpopulation group.

In each of the forty-seven studies, BMR data has been collected for subpopulation groups differentiated by gender, ethnicity, and age. In addition, regression equations have been found corresponding to one or more of the model structures shown in Table 14. As a result, the corresponding reference numbers for different regression models found in each subpopulation are shown in each cell of Table 14. Consequently, in order to find meta-regressions for different categories of regressions and in each subpopulation group, the approach of Bini et al. (2001) is applied. In other words, for the set of studies shown in each cell of the matrix Table 14, the meta-regression formulas described in equation 1 are run to find the combined regression coefficients and standard deviation values. The final results are shown in Table 15. In every subpopulation group, a list of different structures of equations with the corresponding number of studies or regressions is shown. Also, for each row, the range of R^2 – goodness of fit – for that set of studies and the average and standard deviation value is shown in columns 4 and 5.

For example, for the Girls-White- age 5 to 18 years old, four studies have estimated a model with the equation structure 1. The range of R^2 has the minimum 0.48 and the maximum 0.859. Also the average and the standard deviation of R^2, between these four studies, are 0.65 and 0.158, correspondingly. The next few columns show the beta coefficient and the standard deviation (in parentheses) for each independent variable. For example, in the first row the meta-regression found for structure 1, based on four different studies or regressions for girls, white, 5-18 years old, is as follows:

BMR (kcal/d) = 84.7 ($\pm$50.3) + 11.1 ($\pm$0.398) Weight (kg) + 5.46 ($\pm$0.753) Height (cm) -24.8 ($\pm$3.03) Age (years)

Table 14- Summary table of equation structures and populations groups with related studies in each cell

Structure No.	Structure of equation*	Range of R^2	F-T-5-18	M-T-5-18	F-B-4.7-17	M-B-4.7-17	F-P-4-6	M-P-4-6	F-T-18-57	F-T-(>50)	M-T-18-57	M-T-(>50)	F-S-18-50	M-S-18-50	F-B-18-50	F-B-(>50)	M-B-18-50	M-B-(>50)	F-P-(>50)	M-P-(>50)	F-I-18-50	M-I18-50
1	$\beta_0 + \beta_1$ W + β_2 H + β_3 A	0.45-0.86	(Molnar, Jeges, Erhardt, & Schutz, 1995), (Lazzer, Agosti, De Col, & Sartorio, 2006), (Lazzer et al., 2010)	(Molnar, et al., 1995), (Lazzer, et al., 2006), (Lazzer, et al., 2010)					(Bernstein et al., 1983), (Huang, Kormas, Steinbeck, Loughnan, & Caterson, 2004), (Javed et al., 2010), (Lazzer, et al., 2010)	(Bernstein, et al., 1983), (Huang, et al., 2004), (Javed, et al., 2010), (Lazzer, et al., 2010)	(Bernstein, et al., 1983), (Huang, et al., 2004), (Javed, et al., 2010), (Lazzer, et al., 2010)	(Bernstein, et al., 1983), (Huang, et al., 2004), (Javed, et al., 2010), (Lazzer, et al., 2010)	(Ganpule, Tanaka, Ishikawa-Takata, & Tabata, 2007)	(Ganpule, et al., 2007)	(Javed, et al., 2010)	(Javed, et al., 2010)	(Javed, et al., 2010)	(Javed, et al., 2010)				
2	β_4 FFM + β_5 FM		(Garby et al., 1988)	(Garby, et al., 1988)					(Garby, et al., 1988)		(Garby, et al., 1988)											
3	$\beta_0 + \beta_1$ W	0.45-0.90	(Lazzer, et al., 2010)	(Lazzer, et al., 2010)					(Piers, Soares, McCormack, & O'Dea, 1998), (Welle, Forbes, Statt, Barnard, & Amatruda, 1992), (Lazzer, et al., 2010), (Foster, Wadden, & Vogt, 1997)	(Piers, et al., 1998), (Lazzer, et al., 2010)	(Piers, et al., 1998), (Lazzer, et al., 2010)	(Piers, et al., 1998), (Lazzer, et al., 2010)	(Piers & Shetty, 1993)		(Foster, et al., 1997)	(Foster, et al., 1997)	(Dellabianca, Jequier, & Schutz, 1994)		(Aleman-Mateo, Salazar, Hernandez-Triana, & Valencia, 2006)	(Aleman-Mateo, et al., 2006)		
4	$\beta_0 + \beta_4$ FFM + β_5 FM	0.53-0.91							(Bronstein, Mak, & King, 1996), (Soares, Piers, O'Dea, & Collier, 2000), (K. M. Nelson, et al., 1992), (Eric Ravussin & Rising, 1992), (Piers, et al., 1998)	(Weinsier et al., 1995), (Soares, et al., 2000), (K. M. Nelson, et al., 1992), (Eric Ravussin & Rising, 1992), (Piers, et al., 1998)	(Soares, et al., 2000), (K. M. Nelson, et al., 1992), (Eric Ravussin & Rising, 1992), (Piers, et al., 1998)	(Soares, et al., 2000), (K. M. Nelson, et al., 1992), (Eric Ravussin & Rising, 1992), (Piers, et al., 1998)			(Luke et al., 2000)	(Luke, et al., 2000)	(Luke, et al., 2000)	(Luke, et al., 2000)				

5	$\beta_0 + \beta_4$ FFM	0.38-0.92	(Sun et al., 1998), (Kaplan, Zemel, & Stallings, 1996), (DeLany, Bray, Harsha, & Volaufova, 2002), (Lazzer, et al., 2010)	(Sun, et al., 1998), (Kaplan, et al., 1996), (DeLany, et al., 2002), (Lazzer, et al., 2010)	(Sun, et al., 1998), (Kaplan, et al., 1996), (DeLany, et al., 2002)	(Sun, et al., 1998), (Kaplan, et al., 1996), (DeLany, et al., 2002)	(Wren et al., 1997)	(Wren, et al., 1997)	(Welle, et al., 1992), (Jensen, Braun, Vetter, & Marsh, 1988), (Heshka, Yang, Wang, Burt, & Pi-Sunyer, 1990), (Weigle, Sande, Iverius, Monsen, & Brunzell, 1988), (Eric Ravussin & Rising, 1992), (Pannemans & Westerterp, 1995), (Tataranni & Ravussin, 1995), (Lazzer, et al., 2010), (Blanc et al., 2004)	(Lazzer, et al., 2010), (2004), (1995), (Eric Ravussin & Rising, 1992)	(Jensen, et al., 1988), (Heshka, et al., 1990), (Weigle, et al., 1988), (Eric Ravussin & Rising, 1992), (Pannemans & Westerterp, 1995), (Tataranni & Ravussin, 1995), (Lazzer, et al., 2010), (Blanc, et al., 2004)	(Lazzer, et al., 2010), (Blanc, et al., 2004), (Pannemans & Westerterp, 1995), (Eric Ravussin & Rising, 1992)			(Blanc, et al., 2004), (Luke, et al., 2000)	(Blanc, et al., 2004), (Luke, et al., 2000)	(Blanc, et al., 2004), (Luke, et al., 2000), (Dellabianca, et al., 1994)	(Blanc, et al., 2004), (Luke, et al., 2000)				
6	$\beta_0 + \beta_3 A + \beta_4 \log_e FFM + \beta_5 \log_e FM$	0.81-0.81							(J. R. Speakman & K. R. Westerterp, 2010)	(J. R. Speakman & K. R. Westerterp, 2010)	(J. R. Speakman & K. R. Westerterp, 2010)	(J. R. Speakman & K. R. Westerterp, 2010)										
7	$\beta_0 + \beta_3$ A + β_4 FFM + β_5 FM + β_6 WHR									(Luhrmann, Bender, Edelmann-Schafer, & Neuhauser-Berthold, 2009), (Luhrmann, Edelmann-Schafer, & Neuhauser-Berthold, 2010)		(Luhrmann, et al., 2009), (Luhrmann, et al., 2010)										

8	$\beta_0 + \beta_3$ A	0.31-0.33	(Lazzer, et al., 2010)	(Lazzer, et al., 2010)					(Lazzer, et al., 2010)	(Lazzer, et al., 2010), (Luhrmann, et al., 2009), (Luhrmann, et al., 2010)	(Lazzer, et al., 2010)	(Lazzer, et al., 2010), (Luhrmann, et al., 2009), (Luhrmann, et al., 2010)										
9	$\beta_0 + \beta_3$ A + β_4 FFM	0.59-0.77	(Lazzer, et al., 2010)	(Lazzer, et al., 2010)					(Lazzer, et al., 2010), (Huang, et al., 2004)	(Lazzer, et al., 2010), (Huang, et al., 2004), (Blanc, et al., 2004)	(Lazzer, et al., 2010), (Huang, et al., 2004)	(Lazzer, et al., 2010), (Huang, et al., 2004), (2004)				(Blanc, et al., 2004)		(Blanc, et al., 2004)				
10	$\beta_0 + \beta_1$ W + β_3 A	0.41-0.74	(Lazzer, et al., 2010)	(Lazzer, et al., 2010)					(Lazzer, et al., 2010), (De Lorenzo et al., 2000)	(Lazzer, et al., 2010), (De Lorenzo, et al., 2000), (Blanc, et al., 2004)	(Lazzer, et al., 2010), (De Lorenzo, et al., 2000)	(Lazzer, et al., 2010), (De Lorenzo, et al., 2000), (Blanc, et al., 2004)		(Soares, Francis, & Shetty, 1993)		(Blanc, et al., 2004)		(Blanc, et al., 2004)				
11	$\beta_0 + \beta_3$ A + β_4 FFM + β_5 FM	0.43-0.88	(A. M. Tershakovec, K. M. Kuppler, B. Zemel, & V. A. Stallings, 2002), (Lazzer, et al., 2006), (Lazzer, et al., 2010), (Bosy-Westphal et al., 2008)	(A. M. Tershakovec, et al., 2002), (Lazzer, et al., 2006), (Lazzer, et al., 2010), (Bosy-Westphal, et al., 2008)	(A. M. Tershakovec, et al., 2002)	(A. M. Tershakovec, et al., 2002)			(Ferraro, et al., 1992), (Bernstein, et al., 1983), (Eric Ravussin & Rising, 1992), (Bosy-Westphal, et al., 2008), (Hunter, Weinsier, Gower, & Wetzstein, 2001), (Ganpule, et al., 2007), (Gallagher et al., 2006), (Fontvieille, Ferraro, Rising, Larson, & Ravussin, 1993), (Kunz, Schorr, Klaus, & Sharma, 2000), (Lazzer, et al., 2010), (Nielsen et al., 2000), (Wyatt et al., 1999), (Javed, et al.,	(Ferraro, et al., 1992), (Bernstein, et al., 1983), (Eric Ravussin & Rising, 1992), (Bosy-Westphal, et al., 2008), (Hunter, et al., 2001), (Ganpule, et al., 2007), (Gallagher, et al., 2006), (Fontvieille, et al., 1993), (Kunz, et al., 2000), (Lazzer, et al., 2010), (Nielsen, et al., 2000), (Wyatt, et al., 1999), (Javed, et al., 2010)	(Ferraro, et al., 1992), (Bernstein, et al., 1983), (Eric Ravussin & Rising, 1992), (Bosy-Westphal, et al., 2008), (Ganpule, et al., 2007), (Gallagher, et al., 2006), (Fontvieille, et al., 1993), (Kunz, et al., 2000), (Lazzer, et al., 2010), (Nielsen,	(Ferraro, et al., 1992), (Bernstein, et al., 1983), (Eric Ravussin & Rising, 1992), (Bosy-Westphal, et al., 2008), (Ganpule, et al., 2007), (Gallagher, et al., 2006), (Fontvieille, et al., 1993), (Kunz, et al., 2000), (Lazzer, et al., 2010), (Nielsen, et al., 2000), (Wyatt, et al., 1999), (Javed, et al., 2010)			(Gallagher, et al., 2006), (Javed, et al., 2010)	(Gallagher, et al., 2006), (Javed, et al., 2010)	(Gallagher, et al., 2006), (Javed, et al., 2010)	(Gallagher, et al., 2006), (Javed, et al., 2010)			(Fontvieille, et al., 1993)	(Fontvieille, et al., 1993)

									2010)		et al., 2000), (Wyatt, et al., 1999), (Javed, et al., 2010)											
12	$\beta_0 + \beta_3$ A + β_5 FM	0.66-0.66							(Huang, et al., 2004)	(Huang, et al., 2004)	(Huang, et al., 2004)	(Huang, et al., 2004)										
13	$\beta_0 + \beta_3$ A + β_7 BMI	0.65-0.65							(Huang, et al., 2004)	(Huang, et al., 2004)	(Huang, et al., 2004)	(Huang, et al., 2004)										
14	$\beta_0 + \beta_1$ W + β_4 FFM	0.74-0.74							(Horie, Gonzalez, Torrinhas, Cecconello, & Waitzberg, 2011)		(Horie, et al., 2011)											
15	$\beta_0 + \beta_2$ H	0.38-0.41	(Lazzer, et al., 2010)	(Lazzer, et al., 2010)					(Lazzer, et al., 2010)	(Lazzer, et al., 2010)	(Lazzer, et al., 2010)	(Lazzer, et al., 2010)										
16	$\beta_0 + \beta_7$ BMI	0.47-0.47	(Lazzer, et al., 2010)	(Lazzer, et al., 2010)					(Lazzer, et al., 2010)	(Lazzer, et al., 2010)	(Lazzer, et al., 2010)	(Lazzer, et al., 2010)										
17	$\beta_0 + \beta_5$ FM	0.57-0.58	(Lazzer, et al., 2010)	(Lazzer, et al., 2010)					(Lazzer, et al., 2010)	(Lazzer, et al., 2010)	(Lazzer, et al., 2010)	(Lazzer, et al., 2010)										

* Abbreviations- W: Weight (kg); H: Height (cm); A: Age (years); FFM: Fat-Free Mass (kg); FM: Fat Mass (kg); WHR: Waist-to-Hip-Ratio; BMI: Body Mass Index (kg/m^2). F: Female; M: Male; T: White; B: African American; P: Hispanic; S: Asian; I: Pima Native American;

Table 15- Master table including meta-regression equations estimated for different equation structures and population groups. Meta-regression coefficients (standard error) are reported in each cell. Also reported are the number of studies, Range of R^2, and average (Standard Error) of R^2. * Abbreviations- W: Weight (kg); H: Height (cm); A: Age (years); FFM: Fat-Free Mass (kg); FM: Fat Mass (kg); WHR: Waist-to-Hip-Ratio; BMI: Body Mass Index (kg/m^2).

Girls-White- (5-18 years)

Structure No.	Structure of equation	Studies	Range R^2	Average R^2 (SD)	β_0= Intercept	β_1 W*	β_2 H*	β_3 A*	β_4 FFM*	β_5 FM*	β_6 WHR*	β_7 BMI*
1	$\beta_0 + \beta_1$ W + β_2 H + β_3 A	4	0.48 - 0.859	0.65 (0.158)	84.7 (50.3)	11.1(0.398)	5.46 (0.753)	-24.8 (3.03)				
2	β_4 FFM + β_5 FM	3							28.3 (0.824)	6.61 (1.43)		
3	$\beta_0 + \beta_1$ W	1		0.59	901 (73.8)	9.8 (0.72)						
5	$\beta_0 + \beta_4$ FFM	4	0.57 - 0.7	0.625 (0.058)	218 (25.9)				23.9 (1.4)			
8	$\beta_0 + \beta_3$ A	1		0.31	1600 (139)			15.8 (9.6)				
9	$\beta_0 + \beta_3$ A + β_4 FFM	1		0.59	870 (44.5)			-6.69 (3.29)	23.7 (0.837)			
10	$\beta_0 + \beta_1$ W + β_3 A	1		0.59	909 (46)	12 (0.418)		-13.6 (3.41)				
11	$\beta_0 + \beta_3$ A + β_4 FFM + β_5 FM	5	0.47 - 0.79	0.642 (0.12)	513 (33.2)			-7.77 (1.48)	15.4 (1.3)	12.1 (0.819)		
15	$\beta_0 + \beta_2$ H	1		0.41	-708 (327)		15.8 (2.04)					
16	$\beta_0 + \beta_7$ BMI	1		0.47	890 (109)							25.6 (2.93)
17	$\beta_0 + \beta_5$ FM	1		0.58	956 (72.2)					17.4 (1.41)		

Boys-White- (5-18 years)

Structure No.	Structure of equation	Studies	Range R^2	Average R^2 (SD)	β_0= Intercept	β_1 W*	β_2 H*	β_3 A*	β_4 FFM*	β_5 FM*	β_6 WHR*	β_7 BMI*
1	$\beta_0 + \beta_1$ W + β_2 H + β_3 A	4	0.6 - 0.859	0.695 (0.113)	220 (50.5)	11.3 (0.409)	5.82 (0.77)	-25.5 (3.15)				
2	β_4 FFM + β_5 FM	3							29.7 (0.682)	4.37 (2.99)		
3	$\beta_0 + \beta_1$ W	1		0.59	933 (73.8)	12.2 (0.72)						

5	$\beta_0 + \beta_4$ FFM	4	0.47 - 0.7	0.583 (0.0943)	219 (26.2)				25.4 (1.44)			
8	$\beta_0 + \beta_3$ A	1		0.31	848 (139)			94.9 (9.6)				
9	$\beta_0 + \beta_3$ A + β_4 FFM	1		0.59	870 (44.5)			-6.69 (3.29)	23.7 (0.837)			
10	$\beta_0 + \beta_1$ W + β_3 A	1		0.59	1150 (46)	12 (0.418)		-13.6 (3.41)				
11	$\beta_0 + \beta_3$ A + β_4 FFM + β_5 FM	5	0.59 - 0.79	0.678 (0.074)	680 (33.3)			-7.61 (1.49)	16.9 (1.36)	12.8 (0.868)		
15	$\beta_0 + \beta_2$ H	1		0.41	-1320 (327)		21 (2.04)					
16	$\beta_0 + \beta_7$ BMI	1		0.47	639 (109)							41.8 (2.93)
17	$\beta_0 + \beta_5$ FM	1		0.58	954 (72.2)					23.9 (1.41)		
Girls-Black- (4.7-17 years)												
Structure No.	**Structure of equation**	**Studies**	**Range R^2**	**Average R^2 (SD)**	β_0= **Intercept**	β_1**W***	β_2**H***	β_3**A***	β_4**FFM***	β_5**FM***	β_6 **WHR***	β_7 **BMI***
5	$\beta_0 + \beta_4$ FFM	3	0.5 - 0.7	0.57 (0.113)	53.5 (27.5)				29.5 (2.81)			
11	$\beta_0 + \beta_3$ A + β_4 FFM + β_5 FM	1		0.79	-12.5 (53.8)			-15 (7.31)	19.8 (6.4)	7.6 (5.03)		
Boys-Black- (4.7-17 years)												
Structure No.	**Structure of equation**	**Studies**	**Range R^2**	**Average R^2 (SD)**	β_0= **Intercept**	β_1**W***	β_2**H***	β_3**A***	β_4**FFM***	β_5**FM***	β_6 **WHR***	β_7 **BMI***
5	$\beta_0 + \beta_4$ FFM	3	0.51 - 0.7	0.587 (0.1)	55 (27.5)				30 (2.77)			
11	$\beta_0 + \beta_3$ A + β_4 FFM + β_5 FM	1		0.79	111 (53.8)			-15 (7.31)	19.8 (6.4)	7.6 (5.03)		
Girls-Hispanic- (4-6 years)												
Structure No.	**Structure of equation**	**Studies**	**Range R^2**	**Average R^2 (SD)**	β_0= **Intercept**	β_1**W***	β_2**H***	β_3**A***	β_4**FFM***	β_5**FM***	β_6 **WHR***	β_7 **BMI***

5	$\boldsymbol{\beta_0} + \boldsymbol{\beta_4}$ FFM	2	0.384 - 0.792	0.588 (0.288)	28.6 (26.6)				13 (1.63)			
Boys-Hispanic- (4-6 years)												
Structure No.	**Structure of equation**	**Studies**	**Range R^2**	**Average R^2 (SD)**	β_0= **Intercept**	β_1**W***	β_2**H***	β_3**A***	β_4**FFM***	β_5**FM***	β_6 **WHR***	β_7 **BMI***
5	$\boldsymbol{\beta_0} + \boldsymbol{\beta_4}$ FFM	2	0.384 - 0.792	0.588 (0.288)	28.6 (26.6)				13 (1.63)			
Women-White-Young (18-57 years)												
Structure No	**Structure of equation**	**Studies**	**Range R^2**	**Average R^2 (SD)**	β_0= **Intercept**	β_1**W***	β_2**H***	β_3**A***	β_4**FFM***	β_5**FM***	β_6 **WHR***	β_7 **BMI***
1	$\boldsymbol{\beta_0} + \boldsymbol{\beta_1}$ W $+ \boldsymbol{\beta_2}$ H $+ \boldsymbol{\beta_3}$ A	4	0.449 - 0.75	0.619 (0.129)	301 (65.1)	10.2 (0.152)	3.09 (0.385)	-3.09 (0.168)				
2	$\boldsymbol{\beta_4}$ FFM $+ \boldsymbol{\beta_5}$ FM	3							28.3 (0.824)	6.61 (1.43)		
3	$\boldsymbol{\beta_0} + \boldsymbol{\beta_1}$ W	4	0.449 - 0.9	0.645 (0.188)	632 (33.3)	10.9 (0.324)						
4	$\boldsymbol{\beta_0} + \boldsymbol{\beta_4}$ FFM $+ \boldsymbol{\beta_5}$ FM	8	0.526 - 0.91	0.804 (0.15)	360 (29.5)				21 (0.494)	4.68 (0.455)		
5	$\boldsymbol{\beta_0} + \boldsymbol{\beta_4}$ FFM	11	0.53 - 0.922	0.675 (0.115)	473 (15.5)				20.1 (0.43)			
6	$\boldsymbol{\beta_0} + \boldsymbol{\beta_3}\ A + \boldsymbol{\beta_4}\ log_e\ FFM + \boldsymbol{\beta_5}\ log_e\ FM$	1		0.806	-198 (54.8)			-0.299 (0.0968)	149 (48.3)	21.7 (7.01)		
8	$\boldsymbol{\beta_0} + \boldsymbol{\beta_3}$ A	1		0.33	2020 (33)			-5.02 (0.668)				
9	$\boldsymbol{\beta_0} + \boldsymbol{\beta_3}$ A $+ \boldsymbol{\beta_4}$ FFM	2	0.588 - 0.59	0.589 (0.00141)	838 (22.8)			-2.41 (0.176)	19.7 (0.287)			
10	$\boldsymbol{\beta_0} + \boldsymbol{\beta_1}$ W $+ \boldsymbol{\beta_3}$ A	2	0.42 - 0.6	0.51 (0.127)	781 (22)	11 (0.178)		-3.45 (0.232)				
11	$\boldsymbol{\beta_0} + \boldsymbol{\beta_3}$ A $+ \boldsymbol{\beta_4}$ FFM $+ \boldsymbol{\beta_5}$ FM	15	0.425 - 0.88	0.66 (0.136)	682 (25)			-3.08 (0.194)	12.9 (0.47)	5.9 (0.313)		
12	$\boldsymbol{\beta_0} + \boldsymbol{\beta_3}\ A + \boldsymbol{\beta_5}\ FM$	1		0.657	1380 (59.6)			-6.18 (0.744)		11.5 (0.462)		
13	$\boldsymbol{\beta_0} + \boldsymbol{\beta_3}\ A + \boldsymbol{\beta_7}\ BMI$	1		0.647	886 (72.2)			-6.08 (0.742)				26.8 (1.07)
14	$\boldsymbol{\beta_0} + \boldsymbol{\beta_1}\ W + \boldsymbol{\beta_4}\ FFM$	1		0.736	560 (131)	5.39 (2.15)			14.1 (3.73)			
15	$\boldsymbol{\beta_0} + \boldsymbol{\beta_2}$ H	1		0.38	-417 (203)		13.9 (1.18)					

Structure No	Structure of equation	Studies	Range R^2	Average R^2 (SD)	β_0= Intercept	β_1 **W***	β_2 **H***	β_3 **A***	β_4 **FFM***	β_5 **FM***	β_6 **WHR***	β_7 **BMI***
16	$\boldsymbol{\beta_0} + \boldsymbol{\beta_7}$ BMI	1		0.47	794 (53.2)							23.4 (1.28)
17	$\boldsymbol{\beta_0} + \boldsymbol{\beta_5}$ FM	1		0.57	631 (43.4)					21.7 (0.882)		
Women-White-Old (>50 years)												
Structure No	**Structure of equation**	**Studies**	**Range R^2**	**Average R^2 (SD)**	**β_0= Intercept**	**β_1 W***	**β_2 H***	**β_3 A***	**β_4 FFM***	**β_5 FM***	**β_6 WHR***	**β_7 BMI***
1	$\boldsymbol{\beta_0} + \boldsymbol{\beta_1}$ W $+ \boldsymbol{\beta_2}$ H $+ \boldsymbol{\beta_3}$ A	4	0.449 - 0.75	0.619 (0.129)	301 (65.1)	10.2 (0.152)	3.09 (0.385)	-3.09 (0.168)				
3	$\boldsymbol{\beta_0} + \boldsymbol{\beta_1}$ W	2	0.59 - 0.9	0.745 (0.219)	568 (39.1)	11.1 (0.339)						
4	$\boldsymbol{\beta_0} + \boldsymbol{\beta_4}$ FFM $+ \boldsymbol{\beta_5}$ FM	8	0.526 - 0.89	0.751 (0.149)	290 (32.4)				19.9 (0.541)	4.71 (0.466)		
5	$\boldsymbol{\beta_0} + \boldsymbol{\beta_4}$ FFM	4	0.59 - 0.74	0.669 (0.0642)	429 (17.9)				20.9 (0.53)			
6	$\boldsymbol{\beta_0} + \boldsymbol{\beta_3}\, A + \boldsymbol{\beta_4} \log_e FFM + \boldsymbol{\beta_5} \log_e FM$	1		0.806	-198 (54.8)			-0.299 (0.0968)	149 (48.3)	21.7 (7.01)		
7	$\boldsymbol{\beta_0} + \boldsymbol{\beta_3}$ A $+ \boldsymbol{\beta_4}$ FFM $+ \boldsymbol{\beta_5}$ FM $+ \boldsymbol{\beta_6}$ WHR	2			479 (80.6)			-1.99 (0.928)	16.1 (0.606)	6.09 (0.434)	118 (34)	
8	$\boldsymbol{\beta_0} + \boldsymbol{\beta_3}$ A	3	0.33 - 0.33	0.33	1950 (30.5)			-4.72 (0.572)				
9	$\boldsymbol{\beta_0} + \boldsymbol{\beta_3}$ A $+ \boldsymbol{\beta_4}$ FFM	3	0.588 - 0.77	0.649 (0.105)	838 (22.8)			-2.43 (0.175)	19.8 (0.283)			
10	$\boldsymbol{\beta_0} + \boldsymbol{\beta_1}$ W $+ \boldsymbol{\beta_3}$ A	3	0.42 - 0.74	0.587 (0.16)	784 (21.9)	10.9 (0.173)		-3.47 (0.231)				
11	$\boldsymbol{\beta_0} + \boldsymbol{\beta_3}$ A $+ \boldsymbol{\beta_4}$ FFM $+ \boldsymbol{\beta_5}$ FM	15	0.425 - 0.88	0.66 (0.136)	682 (25)			-3.08 (0.194)	12.9 (0.47)	5.9 (0.313)		
12	$\boldsymbol{\beta_0} + \boldsymbol{\beta_3}$ A $+ \boldsymbol{\beta_5}$ FM	1		0.657	1380 (59.6)			-6.18 (0.744)		11.5 (0.462)		
13	$\boldsymbol{\beta_0} + \boldsymbol{\beta_3}$ A $+ \boldsymbol{\beta_7}$ BMI	1		0.647	886 (72.2)			-6.08 (0.742)				26.8 (1.07)
15	$\boldsymbol{\beta_0} + \boldsymbol{\beta_2}$ H	1		0.38	-417 (203)		13.9 (1.18)					
16	$\boldsymbol{\beta_0} + \boldsymbol{\beta_7}$ BMI	1		0.47	794 (53.2)							23.4 (1.28)
17	$\boldsymbol{\beta_0} + \boldsymbol{\beta_5}$ FM	1		0.57	631 (43.4)					21.7 (0.882)		
Men-White-Young (18-57 years)												

Structure No	Structure of equation	Studies	Range R^2	Average R^2 (SD)	β_0= Intercept	β_1W*	β_2H*	β_3A*	β_4FFM*	β_5FM*	β_6 WHR*	β_7 BMI*
1	$\beta_0 + \beta_1$ W + β_2 H + β_3 A	4	0.6 - 0.75	0.671 (0.0619)	522 (65.8)	10.4 (0.156)	3.19 (0.388)	-3.1 (0.169)				
2	β_4 FFM + β_5 FM	3							29.7 (0.682)	4.37 (2.99)		
3	$\beta_0 + \beta_1$ W	2	0.59 - 0.9	0.745 (0.219)	778 (39.1)	11.7 (0.339)						
4	$\beta_0 + \beta_4$ FFM + β_5 FM	7	0.612 - 0.91	0.809 (0.135)	361 (30.8)				21.1 (0.498)	4.77 (0.483)		
5	$\beta_0 + \beta_4$ FFM	10	0.53 - 0.922	0.674 (0.121)	503 (15.6)				18.3 (0.436)			
6	$\beta_0 + \beta_3 A + \beta_4 \log_e FFM + \beta_5 \log_e FM$	1		0.806	-183 (54.8)			-0.299 (0.0968)	149 (48.3)	21.7 (7.01)		
8	$\beta_0 + \beta_3$ A	1		0.33	2640 (33)			-8.37 (0.668)				
9	$\beta_0 + \beta_3$ A + β_4 FFM	2	0.588 - 0.59	0.589 (0.00141)	830 (22.8)			-2.41 (0.176)	19.7 (0.287)			
10	$\beta_0 + \beta_1$ W + β_3 A	2	0.6 - 0.69	0.645 (0.0636)	1050 (22.2)	11 (0.178)		-3.53 (0.236)				
11	$\beta_0 + \beta_3$ A + β_4 FFM + β_5 FM	14	0.45 - 0.88	0.711 (0.208)	898 (27.1)			-3.32 (0.207)	14.3 (0.507)	6.46 (0.374)		
12	$\beta_0 + \beta_3 A + \beta_5 FM$	1		0.657	1930 (59.6)			-6.18 (0.744)		11.5 (0.462)		
13	$\beta_0 + \beta_3 A + \beta_7 BMI$	1		0.647	1440 (72.2)			-6.08 (0.742)				26.8 (1.07)
14	$\beta_0 + \beta_1 W + \beta_4 FFM$	1		0.736	560 (131)	5.39 (2.15)			14.1 (3.73)			
15	$\beta_0 + \beta_2$ H	1		0.38	-1390 (203)		21.3 (1.18)					
16	$\beta_0 + \beta_7$ BMI	1		0.47	985 (53.2)							30.4 (1.28)
17	$\beta_0 + \beta_5$ FM	1		0.57	856 (43.4)					30.4 (0.882)		

Men-White-Old (>50 years)

Structure No	Structure of equation	Studies	Range R^2	Average R^2 (SD)	β_0= Intercept	β_1W*	β_2H*	β_3A*	β_4FFM*	β_5FM*	β_6 WHR*	β_7 BMI*
1	$\beta_0 + \beta_1$ W + β_2 H + β_3 A	4	0.6 - 0.75	0.671 (0.0619)	522 (65.8)	10.4 (0.156)	3.19 (0.388)	-3.1 (0.169)				

3	$\boldsymbol{\beta_0} + \boldsymbol{\beta_1}$ W	2	0.59 - 0.9	0.745 (0.219)	743 (39.1)	11.7 (0.339)						
4	$\boldsymbol{\beta_0} + \boldsymbol{\beta_4}$ FFM + $\boldsymbol{\beta_5}$ FM	7	0.612 - 0.89	0.789 (0.121)	291 (34.3)				20 (0.547)	4.64 (0.497)		
5	$\boldsymbol{\beta_0} + \boldsymbol{\beta_4}$ FFM	4	0.59 - 0.74	0.669 (0.0642)	464 (17.9)				18.6 (0.53)			
6	$\boldsymbol{\beta_0} + \boldsymbol{\beta_3} A + \boldsymbol{\beta_4} \log_e FFM + \boldsymbol{\beta_5} \log_e FM$	1		0.806	-183 (54.8)			-0.299(0.0968)	149 (48.3)	21.7 (7.01)		
7	$\boldsymbol{\beta_0} + \boldsymbol{\beta_3}$ A + $\boldsymbol{\beta_4}$ FFM + $\boldsymbol{\beta_5}$ FM + $\boldsymbol{\beta_6}$ WHR	2			893 (80.6)			-7.06 (0.928)	16.1 (0.606)	6.09 (0.434)	118 (34)	
8	$\boldsymbol{\beta_0} + \boldsymbol{\beta_3}$ A	3	0.33 - 0.33	0.33	2570 (30.5)			-8.29 (0.572)				
9	$\boldsymbol{\beta_0} + \boldsymbol{\beta_3}$ A + $\boldsymbol{\beta_4}$ FFM	3	0.588 - 0.77	0.649 (0.105)	829 (22.8)			-2.43 (0.175)	19.8 (0.283)			
10	$\boldsymbol{\beta_0} + \boldsymbol{\beta_1}$ W + $\boldsymbol{\beta_3}$ A	3	0.6 - 0.74	0.677 (0.0709)	1050 (22.1)	10.9 (0.173)		-3.55 (0.235)				
11	$\boldsymbol{\beta_0} + \boldsymbol{\beta_3}$ A + $\boldsymbol{\beta_4}$ FFM + $\boldsymbol{\beta_5}$ FM	14	0.45 - 0.88	0.711 (0.208)	898 (27.1)			-3.32 (0.207)	14.3 (0.507)	6.46 (0.374)		
12	$\boldsymbol{\beta_0} + \boldsymbol{\beta_3}$ A + $\boldsymbol{\beta_5}$ FM	1		0.657	1930 (59.6)			-6.18 (0.744)		11.5 (0.462)		
13	$\boldsymbol{\beta_0} + \boldsymbol{\beta_3}$ A + $\boldsymbol{\beta_7}$ BMI	1		0.647	1440 (72.2)			-6.08 (0.742)				26.8 (1.07)
15	$\boldsymbol{\beta_0} + \boldsymbol{\beta_2}$ H	1		0.38	-1390 (203)		21.3 (1.18)					
16	$\boldsymbol{\beta_0} + \boldsymbol{\beta_7}$ BMI	1		0.47	985 (53.2)							30.4 (1.28)
17	$\boldsymbol{\beta_0} + \boldsymbol{\beta_5}$ FM	1		0.57	856 (43.4)					30.4 (0.882)		
Women-Asian-Young (18-30 years)												
Structure No	**Structure of equation**	**Studies**	**Range** R^2	**Average** R^2 (SD)	β_0= **Intercept**	β_1**W***	β_2**H***	β_3**A***	β_4**FFM***	β_5**FM***	β_6 **WHR***	β_7 **BMI***
1	$\boldsymbol{\beta_0} + \boldsymbol{\beta_1}$ W + $\boldsymbol{\beta_2}$ H + $\boldsymbol{\beta_3}$ A	1		0.834	-101 (337)	11.5 (1.1)	5.59 (2.01)	-3.3 (0.598)				
3	$\boldsymbol{\beta_0} + \boldsymbol{\beta_1}$ W	1			593 (133)	10.9 (2.72)						
Men-Asian-Young (18-30 years)												
Structure No	**Structure of equation**	**Studies**	**Range** R^2	**Average** R^2 (SD)	β_0= **Intercept**	β_1**W***	β_2**H***	β_3**A***	β_4**FFM***	β_5**FM***	β_6 **WHR***	β_7 **BMI***

1	$\beta_0 + \beta_1 W + \beta_2 H + \beta_3 A$	1		0.834	883 (471)	11.5 (1.1)	5.59 (2.01)	-3.3 (0.598)				
10	$\beta_0 + \beta_1 W + \beta_3 A$	1		0.41	860 (152)	11.6 (1.3)		-3.37 (1.03)				

Women-Black-Young (18-50 yrs.)

Structure No	Structure of equation	Studies	Range R^2	Average R^2 (SD)	β_0= Intercept	β_1W*	β_2H*	β_3A*	β_4FFM*	β_5FM*	β_6 WHR*	β_7 BMI*
1	$\beta_0 + \beta_1 W + \beta_2 H + \beta_3 A$	1		0.675	883 (471)	8.7 (1.4)	-0.342 (2.94)	-3.9 (0.8)				
3	$\beta_0 + \beta_1 W$	1		0.548	302 (148)	13.2 (3.55)						
4	$\beta_0 + \beta_4 FFM + \beta_5 FM$	6	0.75 - 0.84	0.783 (0.0441)	397 (79.5)				20.6 (2.72)	1.9 (0.575)		
5	$\beta_0 + \beta_4 FFM$	4	0.66 - 0.83	0.748 (0.0695)	400 (42)				16.6 (0.949)			
11	$\beta_0 + \beta_3 A + \beta_4 FFM + \beta_5 FM$	3	0.68 - 0.71	0.695 (0.015)	678 (92.8)			-3.28 (0.485)	13.6 (1.16)	5.95 (1.03)		

Women-Black-Old (>50 yrs.)

Structure No	Structure of equation	Studies	Range R^2	Average R^2 (SD)	β_0= Intercept	β_1W*	β_2H*	β_3A*	β_4FFM*	β_5FM*	β_6 WHR*	β_7 BMI*
1	$\beta_0 + \beta_1 W + \beta_2 H + \beta_3 A$	1		0.675	883 (471)	8.7 (1.4)	-0.342 (2.94)	-3.9 (0.8)				
3	$\beta_0 + \beta_1 W$	1		0.548	500 (96.5)	15.6 (1.6)						
4	$\beta_0 + \beta_4 FFM + \beta_5 FM$	6	0.75 - 0.84	0.783 (0.0441)	397 (79.5)				20.6 (2.72)	1.9 (0.575)		
5	$\beta_0 + \beta_4 FFM$	4	0.66 - 0.83	0.748 (0.0695)	400 (42)				16.6 (0.949)			
9	$\beta_0 + \beta_3 A + \beta_4 FFM$	1		0.69	1260 (262)			-11.2 (3.4)	15.9 (5.52)			
10	$\beta_0 + \beta_1 W + \beta_3 A$	1		0.67	1420 (281)	7.6 (0.7)		-11.4 (3.5)				
11	$\beta_0 + \beta_3 A + \beta_4 FFM + \beta_5 FM$	3	0.68 - 0.71	0.695 (0.015)	678 (92.8)			-3.28 (0.485)	13.6 (1.16)	5.95 (1.03)		

Men-Black-Young (18-50 yrs.)

Structure No	Structure of equation	Studies	Range R^2	Average R^2 (SD)	β_0= Intercept	β_1W*	β_2H*	β_3A*	β_4FFM*	β_5FM*	β_6 WHR*	β_7 BMI*

1	$\beta_0 + \beta_1$ W $+ \beta_2$ H $+ \beta_3$ A	1		0.675	1100 (471)	8.7 (1.4)	-0.342 (2.94)	-3.9 (0.8)				
3	$\beta_0 + \beta_1$ W	1		0.63	302 (148)	13.2 (3.55)						
4	$\beta_0 + \beta_4$ FFM $+ \beta_5$ FM	6	0.75 - 0.84	0.783 (0.0441)	421 (82.8)				20.6 (2.72)	1.9 (0.575)		
5	$\beta_0 + \beta_4$ FFM	5	0.66 - 0.83	0.73 (0.0718)	392 (39.1)				17.4 (0.861)			
11	$\beta_0 + \beta_3$ A $+ \beta_4$ FFM $+ \beta_5$ FM	3	0.68 - 0.71	0.695 (0.015)	787 (92.8)			-3.28 (0.485)	13.6 (1.16)	5.95 (1.03)		

Men-Black-Old (>50 yrs.)

Structure No	Structure of equation	Studies	Range R^2	Average R^2 (SD)	β_0= Intercept	β_1W*	β_2H*	β_3A*	β_4FFM*	β_5FM*	β_6 WHR*	β_7 BMI*
1	$\beta_0 + \beta_1$ W $+ \beta_2$ H $+ \beta_3$ A	1		0.675	1100 (471)	8.7 (1.4)	-0.342 (2.94)	-3.9 (0.8)				
4	$\beta_0 + \beta_4$ FFM $+ \beta_5$ FM	6	0.75 - 0.84	0.783 (0.0441)	421 (82.8)				20.6 (2.72)	1.9 (0.575)		
5	$\beta_0 + \beta_4$ FFM	4	0.66 - 0.83	0.748 (0.0695)	400 (42)				16.6 (0.949)			
9	$\beta_0 + \beta_3$ A $+ \beta_4$ FFM	1		0.69	1260 (262)			-11.2 (3.4)	15.9 (5.52)			
10	$\beta_0 + \beta_1$ W $+ \beta_3$ A	1		0.67	1590 (281)	7.6 (0.7)		-11.4 (3.5)				
11	$\beta_0 + \beta_3$ A $+ \beta_4$ FFM $+ \beta_5$ FM	3	0.68 - 0.71	0.695 (0.015)	787 (92.8)			-3.28 (0.485)	13.6 (1.16)	5.95 (1.03)		

Women-Hispanic-Old (>50 yrs.)

Structure No	Structure of equation	Studies	Range R^2	Average R^2 (SD)	β_0= Intercept	β_1W*	β_2H*	β_3A*	β_4FFM*	β_5FM*	β_6 WHR*	β_7 BMI*
3	$\beta_0 + \beta_1$ W	1		0.75	394 (105)	13.6 (1.62)						

Men-Hispanic-Old (>50 yrs.)

Structure No	Structure of equation	Studies	Range R^2	Average R^2 (SD)	β_0= Intercept	β_1W*	β_2H*	β_3A*	β_4FFM*	β_5FM*	β_6 WHR*	β_7 BMI*
3	$\beta_0 + \beta_1$ W	1		0.75	502 (105)	13.6 (1.62)						

Women-Pima Indian (18-50 yrs.)

Structure No	Structure of equation	Studies	Range R^2	Average R^2 (SD)	β_0= Intercept	β_1 W*	β_2 H*	β_3 A*	β_4 FFM*	β_5 FM*	β_6 WHR*	β_7 BMI*
11	$\boldsymbol{\beta_0} + \boldsymbol{\beta_3}$ A + $\boldsymbol{\beta_4}$ FFM + $\boldsymbol{\beta_5}$ FM	1		0.88	705 (60.3)			-2.2 (0.8)	15 (1.1)	4.4 (0.7)		
Men- Pima Indian (18-50 yrs.)												
Structure No	**Structure of equation**	**Studies**	**Range R^2**	**Average R^2 (SD)**	**β_0= Intercept**	**β_1 W***	**β_2 H***	**β_3 A***	**β_4 FFM***	**β_5 FM***	**β_6 WHR***	**β_7 BMI***
11	$\boldsymbol{\beta_0} + \boldsymbol{\beta_3}$ A + $\boldsymbol{\beta_4}$ FFM + $\boldsymbol{\beta_5}$ FM	1		0.88	829 (60.3)			-2.2 (0.8)	15 (1.1)	4.4 (0.7)		

5. Conclusions and Future Research

This study is the most comprehensive systematic literature review performed to estimate reliable equations for predicting Basal Metabolic Rate (BMR). In this approach, a meta-analysis method is applied which required the standard deviation estimates of all regression coefficients. Unfortunately, only 19% of the studies found (i.e., forty-seven) reported the required statistic for our analysis, and the rest were excluded from further analysis.

In order to compare the regression models, each subpopulation is considered separately. In regards to the 'Girls-White- (5-18 years)', three structures, including 1 (i.e., β_0 + β_1 W + β_2 H + β_3 A), 2 (i.e., β_4 FFM + β_5 FM), 5 (i.e., β_0 + β_4 FFM) and 11 (i.e., β_0 + β_3 A + β_4 FFM + β_5 FM), are the results of combining 3 or more studies, which makes them more robust. Although structure 5 has a higher average R^2 (i.e., 0.625), and the Fat-Free Mass factor has often been cited as the best independent predictor of BMR (Cunningham, 1991), additional determinants have been suggested to be included in the model for predicting BMR. Overall, we suggest applying either regression structures 1, 2 or 11, since above and beyond the Fat-Free Mass, they also include the Fat Mass factor (structures 2 and 11) or include weight and height terms together (structure 1), which is more comprehensive. However, structures 1 and 11 also include the age factor, which in most cases negatively influences BMR (meaning as the individual gets older, the BMR decreases). This model is extremely beneficial for considering the time dependence of Basal Metabolic Rate (BMR) in the dynamic energy balance models. Also, both these structures have a higher average R^2, while for structure 2, the R^2 is not reported. The same analysis holds for 'Boys-White- (5-18 years),' and we suggest applying either structure 1 or 11 for predicting BMR in this subpopulation as well.

In regards to the subpopulation Girls or Boys-Black (4.7-17 years), structure 5 is based on 3 studies and more robust; nevertheless, structure 11 includes Fat-Mass and has a higher average R^2. For Hispanic Boys or Girls, 4-6 years, only one structure is found.

In the subpopulation 'Women-White-Young (18-57 years)', the structures which are a combination of more than one study, including structures 1 (i.e., β_0 + β_1 W + β_2 H + β_3 A), 2 (i.e., β_4 FFM + β_5 FM), 3 (i.e., β_0 + β_1 W), 4 (i.e., β_0 + β_4 FFM + β_5 FM), 5 (i.e., β_0 + β_4 FFM), 9 (i.e., β_0 + β_3 A + β_4 FFM), 10 (i.e., β_0 + β_1 W + β_3 A) and 11 (i.e., β_0 + β_3 A + β_4 FFM + β_5 FM), are more robust. Among them structures 4, 5 and 11 have higher average R^2. However, structures 4 and 11 are more comprehensive, (i.e., include both factors FFM and FM). Between these two structures, structure 4 has a much higher average R^2, but structure 11 also includes the age factor (i.e., BMR decreases with advancing age). Both structures 4 and 11 are suggested to be applied for this subpopulation. The same holds for 'Men-White-Young (18-57 years)', 'Women-White-Old (>50 years)' and 'Men- White-Old (>50 years)'.

In the Asian-Young subpopulation, for both men and women, structure 1 is suggested, because of higher average R^2. In the Black-Young and old subpopulations of men and women, structures 4 and 11 are also suggested to be used. Both have higher R^2 and cover more significant determinants (both FM and FFM factors) and also the age factor. In the Hispanic and Pima-Indian subpopulations, only one structure is found.

In conclusion, several models for different subpopulations are found which describe the dependence of BMR on age and body measures including body weight, body mass index, Fat Mass and Fat-Free Mass. As shown in matrix Table 14, most of the studies have found equations for structures 4, 5 and 11. Also, among all subpopulations, the white population including children, adolescents and adults (young and old), and then the adult black population are studied more frequently.

Overall, we can observe based on the final meta-regression models found in this research, that the most important independent factors based on frequency of usage in the model for predicting BMR, include the constant term, followed by FFM or Age, and then Weight or FM. Also, all the models show a positive relation between BMR and body measure factors, and the Fat-Free Mass term has a higher Basal Metabolic Rate than the Fat Mass. This indicates that the overweight and obese people would have a higher BMR than the lean ones. However, by applying these prediction models, BMR can be included as an endogenous variable in the dynamic energy balance model of projecting body weight dynamics. The robust predictions of BMR would lead to more reliable estimations of total energy expenditure and then the changes of body weight over the lifecycle of the human body. This would lead to a more accurate discussion regarding the relation of obesity and BMR, regarding which differences of opinions exist, for example, about the energy efficiency of obese and lean subjects.

In almost in all models, the relation of BMR to Age is negative, except for in structure 8 (i.e., β_0 + β_3 A), where the model includes only the factor 'Age', with a positive coefficient for all subpopulations. This is likely because of increasing weight by age during adulthood. It seems that the common belief in the literature, that BMR is declining with age, cannot be rejected based on our results, and also it is not approved that BMR does not change with advancing age (Roza & Shizgal, 1984). Furthermore, the meta-analysis results show that the sign of the age term does not change from young ages (i.e., < 50 years) to the old ages (i.e., above 50 years) in any of the models for different subpopulations, contrary to Speakman and Westerterp's (2010) findings.

As future steps, in order to compare the validity and effectiveness of various BMR predicting equations, we need to obtain a dataset including all predicting factors and the corresponding BMR values. Then we can apply different approaches for comparing the models, such as Bland-Altman analysis (Bland & Altman, 1986), finding the proportion of predicted BMRs falling within a certain distance of the measured BMR, root mean square deviation (RMSD), mean absolute error (MAE), mean absolute percentage error (MAPE), or the statistical significance of differences observed between predicted and measured BMR values .

Also, it is possible to find weighted averages of all the meta-regression formulas for each subpopulation, which will be used to create a set of benchmark synthetic data for BMR, using the corresponding data on determinants such as weight, height, and body composition already available in data sets such as the National Health and Nutrition Examination Survey (NHANES). Such synthetic data can then be used to estimate a more comprehensive regression model. Furthermore as an alternative approach, the R^2 – goodness of fit – reported for each regression can be used to find other weighted averages of regressions.

Third Essay - References

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Appendix A:

Coding Details

A sample of detailed coding for one of the studies by Molnar et al (1995) is reported. Some of the fields (e.g. Mean Age) were not reported in the paper, and so are empty.

Table A.1- Coding of the data set

Data Key	Source Reference for Data	Reference Key	Sample Size	Random or Opportunistic	Ethnicity	Location of Study	Min Age (years)	Max Age years)	Mean Age (years)	No. of Female	No. of Male	Obese-Male	Obese-Female	Non-Obese Male	Non-Obese Female	BMI Range
1	1	1	371	Opportunistic	Caucasian	Pecs/ Hungary	9.5	16.5		178	193	77	59	116	119	

Table A.2-Coding of the Prediction Equations

Indicator*	Equation Key	Reference Key	Size (n)	Data Key	Subpopulation		Dependent Variable						Model	Purpose	Finding/ Formula	Correlation Table-Independent Variables (Yes/No)	Correlation Table-Beta (Yes/No)	Goodness of Fit						Independent Variables					
																								Intercept					...
					Full Sample	Specify	Method	Description	Body Composition Measurement Method	Time of Day	Name	Unit						R^2	Adjusted R^2	MSE	RMSE	p-value	SEE	Beta	Variance (Beta)	t-stat	p-value	Approximate?	...
1	1	1	371	1	Yes		RMR	Deltatrac metabolic cart using the ventilated hood technique for 45 min. From measured oxygen uptake and CO2 output based on Lusk formula. After overnight fast at 7:30 a.m.	Relative body fat was estimated from five skin-fold thicknesses according to Parizkova and Roth. Lean body mass was calculated by subtracting body fat mass (i.e., the percentage body fat x body weight) from body weight.	Morning After Overnight Fasting	BMR	KJ	Y=BetaX+e	Validity of five predictive equations for RMR was studied and new predictive equations found. The new equations were validated against new data set.	RMR(kJ/24hr) = 50.2 Weight(kg)+ 29.6Height (cm) -144.5Age(yr) - 550Sex + 594.3 (R^2=0.859, p<0.001)	No	No	0.859						594.3	36985.3049		0.001	Yes	

* Indicator is 2, if the standard deviation of the beta coefficient is already reported in the study, or 1, if it is estimated based on the p-values or t-stat reported, and 0, if it is estimated based on the p-value significance level of comparing the intercept value of the regressions found for different groups.

Appendix B:

Procedures to extract/estimate variance or standard deviation of reported regression parameters based on p-value or t-statistic

'Indicator' field in Table S.2, identifies the studies that report the variance of the regression coefficients (Indicator=2) directly, vs. those that report the p-value or t-statistic instead (Indicator=1). We calculate the coefficient standard deviation for this latter category. For any regression coefficient, in determining the significance level associated with the difference of the estimated coefficient with a threshold value of β_0, the following formula is used:

$$t_{\hat{\beta}} = \frac{\hat{\beta} - \beta_0}{Standard\ Error(\hat{\beta})} \qquad (Equation\ 1)$$

Usually the t-statistic is reported for $\beta_0=0$, so the following formula is used in finding the standard deviation:

$$Standard\ Deviation\ (\hat{\beta}) = \frac{\hat{\beta}}{t_{\hat{\beta}}} \qquad (Equation\ 2)$$

In some cases, only the p-value significance level associated with the t-statistic is reported. In those cases, first the corresponding t-statistic for that p-value is found (from T or Normal distribution table) and then the above formula is applied. When only the upper bound of the p-value is reported (e.g. p-value<=0.001), then it is assumed (conservatively) that the p-value is equal to the upper bound. For example, if the regression model finds

$$\hat{\beta} = 594.3$$

and p-value <=0.001, with a sample size greater than 30 (so normal distribution can be assumed), then the t-statistic is assumed to equal the inverse of standard normal distribution with cumulative probability of 0.001, i.e. 3.09. This leads, conservatively, to a standard deviation of 192.3 for this coefficient.

In some studies different regression equations have been reported for different population groups but significance levels are aggregate (Indicator=0). As an example we consider, DeLany, Bray, Harsha, and Volaufova [55] who report on African-Americans (sample size: n_1=65): BMR(MJ/d)=0.157Fat-Free Mass +1.365 (R^2=0.51, p<0.0001), and Whites (sample size: n_2=66):

BMR(MJ/d)=0.204 Fat-Free Mass +0.310 (R^2=0.57, p<0.0001). Yet they report the p-value for checking the significance of all the regression coefficients at the same time, which in this case, there is only one determinant, and so the p-value<0.0001, is corresponding to the Fat-Free Mass factor for both groups. To find the standard deviation for the intercept, the authors also report that based on the results of ANOVA, the differences in intercepts of regressions for African Americans and Whites has a p-value<0.05. On the other hand the standard error of the total sample is equal to the following:

$$\sqrt{\frac{{\sigma_1}^2}{n_1}+\frac{{\sigma_2}^2}{n_2}}$$

It is already known that:

$$\frac{\mu_1-\mu_2}{\sqrt{\frac{{\sigma_1}^2}{n_1}+\frac{{\sigma_2}^2}{n_2}}}=t\_stat_{p\_value}$$

Also,

$$\left(Intercept_{African\ -American}\ -Intercept_{White}\right)=1.055$$

and assuming that,

$$\sigma_1=\sigma_2=\sigma$$

then the following is found:

$$\frac{(\mu_1-\mu_2)}{t\_stat_{p<0.05}\sqrt{\frac{1}{n_1}+\frac{1}{n_2}}}=\sigma$$

Finally for each sample, σ^2 needs to be divided by the corresponding sample size. So for African-Americans, the standard error of the intercept is equal to $\sigma/\sqrt{65}$ =0.455 and for Whites, is equal to $\sigma/\sqrt{66}$ = 0.452.

Appendix C: The first category of studies identified from the Systematic Review, include those that predict a Basal Metabolic Rate equation based on an empirical dataset, but lack enough detail to allow analytical meta-regression. The full list including 201 studies are as below:

1 Alfonzo-Gonzalez G, Doucet E, Bouchard C, Tremblay A. Greater than predicted decrease in resting energy expenditure with age: cross-sectional and longitudinal evidence. *Eur J Clin Nutr*. 2006; 60: 18-24.

2 Arciero PJ, Tyzbir RS, Goran MI, Poehlman ET. Prediction of Resting Metabolic-Rate in Older Men. *Clin Res*. 1992; 40: A204-A04.

3 Arciero PJ, Goran MI, Gardner AM, Ades PA, Tyzbir RS, Poehlman ET. A Practical Equation to Predict Resting Metabolic-Rate in Older Females. *J Am Geriatr Soc*. 1993; 41: 389-95.

4 Arciero PJ, Goran MI, Poehlman ET. Resting Metabolic-Rate Is Lower in Women Than in Men. *J Appl Physiol*. 1993; 75: 2514-20.

5 Arciero PJ, Goran MI, Gardner AW, Ades PA, Tyzbir RS, Poehlman ET. A Practical Equation to Predict Resting Metabolic-Rate in Older Men. *Metab-Clin Exp*. 1993; 42: 950-57.

6 Astrup A, Thorbek G, Lind J, Isaksson B. Prediction of 24-h energy expenditure and its components from physical characteristics and body composition in normal-weight humans. *Am J Clin Nutr*. 1990; 52: 777-83.

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