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# A Study on Network Design Problems for Multi-modal Networks by Probitbased Stochastic User Equilibrium

Kenetsu Uchida<sup>a</sup>, Agachai Sumalee<sup>b\*</sup>, David Watling<sup>b</sup>, Richard Connors<sup>b</sup>

<sup>a</sup> Graduate School of Engineering, Hokkaido University

<sup>b</sup> Institute for Transport Studies, University of Leeds

\* Corresponding author. 36 University Road, Leeds, LS2 9JT, UK Tel: +44-113-343-5345;

Fax: +44-113-343-5334.

E-mail address: asumalee@its.leeds.ac.uk

**Abstract.** This paper develops a multi-modal transport network model considering various travel modes including railway, bus, auto, and walking. Travellers are assumed to choose their multi-modal routes so as to minimise their perceived disutilities of travel following the Probit Stochastic User Equilibrium (SUE) condition. Factors influencing the disutility of a multi-modal route include actual travel times, discomfort on transit systems, expected waiting times, fares, and constants specific to transport modes. The paper then deals with the multi-modal network design problem (NDP). The paper employs the method of sensitivity analysis to define linear approximation functions between the Probit SUE link flows and the design parameters, which are then used as constraints in the sub-problem of the NDP instead of the original SUE condition. Based on this reformulated NDP, an efficient algorithm for solving the problem is proposed in the paper. Two instances of this general NDP formulation are then presented in the paper: the optimal frequency design problem (AADP).

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#### 1. Introduction

The improvement or modification of a transport network and service often requires a high level of investment. With limited public funds, it is important to carefully evaluate the costs and potential benefits of different transport schemes. Transport network models have long been used as a decision support system for the decision-maker in evaluating potential benefits and impacts of different transport projects. This is one way of using a model, as an *ad hoc* tool.

It is also possible to use the model to directly identify the best (optimal) way to modify the transport network/service. This problem is widely referred to as the Network Design Problem (NDP). The NDP for the case of automobile-only networks has been widely studied in the literature (see for example Abdulaal and LeBlanc 1979; Tobin and Friesz 1988; Yang and Bell 1997; Shepherd and Sumalee 2004). The NDP is normally formulated as a Mathematical Program with Equilibrium Constraints (MPEC) in which the planner aims to define modifications to a network so as to optimise an objective function, whilst considering the response of travellers to the changes following an equilibrium condition. Often, the travellers' responses are assumed to follow Wardrop's User Equilibrium condition (UE).

The NDP is not only applicable to the case of the road network. It can also be used to analyse transit network planning or in a more general multi-modal network case. Note that public transport users are believed to be more strategic (than those in an automobile network) in choosing their routes or service lines, depending on the arrival of services at the boarding point or the expected waiting time (Chiriqui and Robillard 1975). At the tactical level, the design parameters involved in the NDP of the transit network may include service line, service frequency and fare level and structure. Most of the works reported in the literature related to the NDP of a transit network simply ignore the response of travellers to the change or configuration of the transit network or service (Gao *et al* 2004).

Gao *et al* (2004) pointed out this pitfall of previous studies and proposed a formulation of a continuous NDP of transit systems with the UE model for transit network assignment. The transit assignment model adopted in Gao *et al* (2004) is similar to the one

proposed in De Cea and Fernandez (1993), an extension of the model proposed by Spiess and Florian (1989) to consider the impact on waiting delay of limited vehicle capacities. In this paper we aim to apply the NDP with a more advanced framework of the multi-modal network as compared to the one adopted in Gao *et al* (2004). In this respect, the main improvements in the model adopted for the NDP in this paper are fourfold.

First, we extend the analysis of the NDP to the case of a multi-modal network in which a single journey may comprise more than one mode (see e.g. Fernandez *et al* 1994; Lo *et al* 2003). Second, the model adopted in this paper allows some public transport modes to share the road space with the private automobile. Thus, their travel times on the road network are interrelated with traffic volumes and *vice versa*. This is particularly important for the optimal frequency design problem since a large increase in bus frequency may ultimately cause some major travel delays on some links. Third, we introduce an in-vehicle "congestion effect" in addition to the waiting time. This is mainly to represent the discomfort or crowding effect on public transport passengers, which may influence travellers' behaviour (Kraus 1991). Similar to the model proposed in this paper, Kurauchi *et al* (2003) propose a transit assignment model with a nonlinear crowding effect.

Lastly, the framework of probit Stochastic User Equilibrium (SUE) is adopted instead of UE. The concept of SUE is believed to be a more plausible model than UE in allowing for mis-perceptions and uncertainties in travellers' predictions of travel disutilities. It has also been shown that it can eliminate some problems in solving the NDP caused by the UE condition (Lawphongpanich and Hearn 2004; Sumalee *et al* 2005). Several previous researchers have also applied SUE to the case of a public transport network model. Lam *et al* (1999) introduced line capacity constraints to a logit-based SUE transit assignment for a congested transit network. Lo *et al* (2003) also adopted the logit SUE model to represent passengers' route choice behaviours. Nielsen (2000) presented a framework for transit assignment that builds on a probit-based SUE model that resolves the problem with overlapping routes in the logit-model, caused by its IIA (independence of irrelevant alternatives) condition. Apart from these four improvements to the multi-modal model in the NDP context, this paper also presents a new application of the NDP with the optimal anti-freezing admixture dispersion problem, in addition to the optimal frequency design problem. The paper is structured into seven further sections.

The next section introduces the representation of a multi-modal network. Then in Section 3, the probit-based SUE formulation for passengers' route choice in the multi-modal network is explained. This section also gives details of the definition and formulation of the different components of disutility of travel on a multi-modal route. Two network design problems of optimal transit frequency design (FDP) and optimal anti-freezing admixture dispersion (AADP) are formulated in Section 5. Then, Section 6 proposes a solution algorithm for the NDP. Section 7 then discusses the numerical examples and Section 8 concludes the paper and discusses future research needs.

#### 2. Network Representation

First, some definitions will be made in order to explain the network representation. A *transit line* (or just a *line*) is a group of vehicles that runs back and forth between two nodes on a transit network. A *line section* is any portion of a transit line between two (not necessarily consecutive) nodes of its itinerary. Figure 1a shows a simple example of the primitive network taken from Spiess and Florian (1983). There are four lines in this network (L1-L4). This primitive network is transformed into a modified network shown in Figure 1b, i.e. G(N,S) with node set N representing transit stops and link set S representing *route sections*. A *route section* is a portion of a route between two consecutive transfer nodes. A *route* is any path that a transit user can follow on the transit network to travel between any two nodes. In Figure 1b, each route section is associated with a set of attractive lines characterizing expected travel time on that route section. The set of attractive lines on route section s, i.e.  $\overline{A}^s$ , can be determined by solving the following problem.

$$\min_{\{x_l^s\}} Z^s = \frac{60\alpha + \sum_l \bar{t}_l^s f_l x_l^s}{\sum_l f_l x_l^s}$$
(1)

s.t.

$$x_{l}^{s} = 0, 1 \ \forall l \in A^{s}, f^{s} = \sum_{l} f_{l} x_{l}^{s},$$
 (2)

where,  $A^s$ ,  $f_l$  and  $\bar{t}_l^s$  denote a set of all transit lines passing through route section *s*, the frequency of transit line *l* (services/hr) and the constant in-vehicle travel time (min.) of route section *s* using transit line *l* respectively. The objective function as defined in Eq.(1) denotes the total expected travel time, i.e. the expected waiting time plus the expected in-vehicle travel time, calculated using frequencies and constant in-vehicle travel times of transit lines on route section *s*. The effect of both the distribution of headway times of the transit lines and the distribution of passenger arrival times on the calculation of the expected waiting time is captured by the parameter  $\alpha$  in Eq.(1).

#### [INSERT FIGURE 1]

The case  $\alpha = 1$  corresponds to an exponential distribution of interval times of the transit lines with mean  $1/f^s$  and a uniform passenger arrival rate. The case  $\alpha = 1/2$  is an approximation of a constant headway time  $1/f^s$  for the transit lines. A line  $l \in A^s$  will be included in a set of attractive lines ( $\overline{A}^s$ ) for route section *s* if  $x_l^s = 1$ , and will not be considered as a possible line if  $x_l^s = 0$ .

In this paper, the multi-modal network is expressed as a hyper-network, i.e. the road network including the walking network plus the modified network representing the transit network as mentioned above. Links for auto or walking can be considered as links used by the L+1th dummy line where L denotes the number of real lines in the multi-modal network with frequencies and service capacities of infinity, i.e. a waiting time and in-vehicle discomfort of zero. Based on this idea, we will denote transit stops and route sections as nodes and links respectively, without distinguishing nodes and links comprising the road network. In reality,



(a) Primitive network and its itinerary.



(b) Modified transit network.

Fig. 1. Network representation for the transit network.

autos and buses may share the same road space and this is represented in the hyper-network by using two different links having interactions with each other in terms of the congestion effect. However, the delay on the pseudo-link representing a bus line also includes the invehicle congestion effect (expected waiting time). The link set of the hyper-network will be comprised of four subsets associated with the four transport modes.

$$S= \underset{m\in \{w,a,b,u\}}{\cup} S_m$$

where *m* indicates transport modes for walking (m=w), auto (m=a), bus (m=b) and subway (m=u), and  $S_m$  indicates a set of links in which the transport mode is *m*. Henceforth, we will denote by *s* an element of the set *S* when we do not have to distinguish transport modes.

#### 3. Link Disutility Functions

#### 3.1. Notation

The notation adopted in this paper is shown below:

- *S* The number of links comprising the multi-modal network.
- *L* The number of real lines in the multi-modal network
- A  $(S \times L+1)$ -matrix that has an element  $a_{sl}$ , representing the sth row and  $l^{\text{th}}$  column of A; equal to 1 if link s includes a line l as one of its attractive lines, and 0 otherwise
- $\overline{A}^s$  The set of lines that are included in link *s* as attractive lines
- V S-vector of link flows, having  $s^{\text{th}}$  element  $V^s$  denoting the number of passengers on link s
- **v**  $(S \times L+1)$ -matrix that has an element  $v_{sl}$ , representing the  $s^{\text{th}}$  row and  $l^{\text{th}}$  column of **v**, that denotes the number of passengers on link *s* using line  $l(V^s = \sum_{l} v_{sl})$ .
- $\tilde{v}_{sl}$  The number of passengers that share the same line *l* with the passengers on link *s* using line *l* ( $v_{sl}$ )
- $\widetilde{V}^{s}$  The number of passengers that share the same link with the passengers on link  $s(V^{s})$ ,  $(\widetilde{V}^{s} = \sum_{l \in \overline{A}^{s}} \widetilde{v}_{sl})$
- **f** (L+1)-vector of line frequencies that has an element  $f_l$ , representing the  $l^{\text{th}}$  element of **f**, which denotes the frequency of line l (services/hr.)
- $\kappa$  (*L*+1)-vector of service capacities that has an element  $\kappa_l$ , representing the *l*<sup>th</sup> element of  $\kappa$ , which denotes vehicle capacity comprising a service of the transit line *l* (passengers/service)
- t<sup>\*</sup> S-vector of actual travel times that has an element  $t^{*s}$ , representing  $s^{th}$  element of t<sup>\*</sup>; equal to 0 if  $s \in S_h$ , and  $\bar{t}^s$  otherwise, where  $\bar{t}^s$  denotes actual travel time of link s
- $\hat{\mathbf{t}}$  S-vector of perceived travel time that has entries  $\hat{t}^s$  representing the  $s^{\text{th}}$  element of  $\hat{\mathbf{t}}$ , which denotes the perceived travel time of link s.
- **d** S-vector of link disutilities with  $d^s$  representing disutilities of link s.

- **w** S-vector of link expected waiting time with  $w^s$  representing expected waiting time of link s.
- **p** S-vector of fares on links with entries  $p^s$  representing the fare on link s.
- Ω (S × S)-matrix that has an element  $ω_{ss'}$ , representing the s<sup>th</sup> row and s'<sup>th</sup> column of Ω; equal to 1 if in-vehicle congestion on link s is affected by the number of passengers on link s', and 0 otherwise
- **J**  $(S \times L+1)$ -matrix that has an element  $j_{sl}$ , representing the  $s^{th}$  row and  $l^{th}$  column of **J**; equal to 1 if link *s* is a *direct link* regarding line *l*, and 0 otherwise, where if the passengers travelling on link *s* using line *l* cannot alight from the line along the way, we call link *s* a *direct link* regarding line *l*
- **H**  $(S \times L+1)$ -matrix that has an element  $h_{sl}$ , representing  $s^{th}$  row and  $l^{th}$  column of **H**; equal to 1 if line l passes through link s in the original network, and 0 otherwise for  $s \in S_a$  and  $l \neq L+1$ ; equal to 1 for  $s \in S_a \cup S_w$  and l=L+1; equal to 0 for  $s \in S_w$  and  $l \neq L+1$ ; equal to 0 for  $s \in S_b$  and  $\forall l$ ; and equal to  $a_{sl}$  for  $s \in S_u$  and  $\forall l$
- **E**  $(S \times S)$  matrix that has an element  $e_{ss'}$ , representing the  $s^{th}$  row and  $s^{th}$  column of **E**; equal to 1 if s = s', and 0 otherwise for  $s \in S_b$ ; and equal to 1 if actual travelling time on link s is affected by the number of passengers on link  $s' \in S_a$ , i.e. equal to 1 in the case where bus link s shares auto link s' in the original network, and 0 otherwise
- $\mathbf{1}_{S}$  S-vector whose elements are all equal to 1
- $\mathbf{1}_{L+1}$  (L+1)-vector whose elements are all equal to 1

In this paper, the arithmetic signs of  $\otimes$  and  $\div$  indicate the special operations of element-by-element multiplication and division for matrices or vectors, respectively. For example, element-by-element multiplication of matrices of **M** and **N** is written as **M**  $\otimes$  **N** in which the element in the *i*<sup>th</sup> row and *j*<sup>th</sup> column of the matrix **M**  $\otimes$  **N** is  $m_{ij} n_{ij}$ , where  $m_{ij}$  and  $n_{ij}$  indicate the elements in the *i*<sup>th</sup> row and *j*<sup>th</sup> column of **M** and **N** respectively. The arithmetic sign of  $\div$  indicates element-by-element division of matrices or vectors, such that **M**  $\div$  **N** has an element in the *i*<sup>th</sup> row and *j*<sup>th</sup> column of  $m_{ij}/n_{ij}$ . Note that, two matrices (or vectors) used for two arithmetic signs of  $\otimes$  and  $\div$  should have the same size. The superscript *T* denotes the conventional matrix transposition operator.

#### 3.2 Disutility of link and intermodal route

In this paper, the travellers are assumed to consider four main components of the inconvenience or disutility of travel on a link or route, explicitly including travel time, invehicle congestion effect, expected waiting time, and fares. As we will explain later in the next section, the in-vehicle congestion effect (crowding effect) and travel time can be

combined as a perceived travel time. Thus, in general the total disutility of using hyper link *s* in the intermodal network as described in the previous section can be defined as:

$$\mathbf{d} = \boldsymbol{\pi} \otimes \hat{\mathbf{t}} + \boldsymbol{\rho} \otimes \mathbf{w} + \boldsymbol{\tau} \otimes \mathbf{p}, \qquad (3)$$

$$d^{s} = \pi^{s} \hat{t}^{s} + \rho^{s} w^{s} + \tau^{s} p^{s} \quad \forall s,$$

$$\tag{4}$$

, following the notation defined in the previous section, where  $\pi$ ,  $\rho$ , and  $\tau$  denote coefficients vectors (all with the size of  $|S| \times 1$ ) on the perceived travel times vector, waiting times vector and fares vector, respectively

Then, the disutility function of an intermodal route can be defined as the sum of the related link disutilities with an additional term of a mode specific constant (or alternative specific constant, ASC). The disutility of the  $k^{th}$  intermodal route connecting origin node r and destination node s, i.e. the  $k^{th}$  intermodal route between OD pair rs, is given by:

$$du_k^{rs} = \sum_{m \in \{w,a,b,u\}} \alpha^m \zeta_{m,k}^{rs} + \sum_{s \in S} d^s \delta_{s,k}^{rs} \quad \forall k \in K_{rs}, \forall rs ,$$
(5)

where,  $\alpha^m$  denotes the mode specific constant for mode *m*. For a  $k^{th}$  intermodal route between OD pair *rs*  $\zeta_{m,k}^{rs} = 1$  if it contains at least a link whose transport mode is *m* and  $\delta_{s,k}^{rs} = 1$  if it is related to link *s*. Otherwise,  $\zeta_{m,k}^{rs}$  or  $\delta_{s,k}^{rs}$  is 0. The set of intermodal routes connecting OD pair *rs* is  $K_{rs}$ . The monetary costs of auto are mainly due to car ownership costs, fuel costs, and tolls. The car ownership cost is reflected by the mode-specific constant for auto.

It is noted that a number of previous studies have also considered the impact on the disutility of a trip of modal transfers (see for example Lo *et al*, 2003). In the present study, the disutility from the number of modal transfers will not be modelled explicitly, because it can also be represented implicitly inside the expected waiting time and walking travel time.

As explained later in Section 3.4 and 3.5, the formulations of perceived in-vehicle travel time (with the crowding effect) and the expected waiting time are functions of two types of passenger flows. First, they are functions of the number of passengers already on-board, which obviously influences the level of in-vehicle congestion for each service line and the capacity remaining for additional passengers. Second, they are functions of the number of

passengers wishing to board and alight at different stations. The definitions and mathematical formulation in matrix form will be explained next.

#### 3.3 Formulation of passenger volumes

For the passenger volume using line l on link  $s(v_{sl})$  can be simply defined in a matrix format as:

$$\mathbf{v} = (\mathbf{A} \operatorname{diag}(\mathbf{f})) \otimes (\mathbf{P} \mathbf{1}_{L+1}^T)$$
(6)

where

$$\operatorname{diag}(\mathbf{f}) = \begin{pmatrix} f_1 & \cdots & 0\\ \vdots & \ddots & \vdots\\ 0 & \cdots & f_{L+1} \end{pmatrix},$$
(7)

$$\mathbf{P} = \mathbf{V} \otimes \left\{ \mathbf{l} \div (\mathbf{A}\mathbf{f}) \right\}$$
$$= \begin{pmatrix} V^1 / (\sum_{l \in \overline{A}^1} f_l) \\ \vdots \\ V^S / (\sum_{l \in \overline{A}^s} f_l) \end{pmatrix}.$$
(8)

The element representing the  $s^{th}$  row and  $l^{th}$  column of **v** is given by:

$$v_{sl} = V^{s} \left( f_{l} / \sum_{l' \in \overline{A}^{s}} f_{l'} \right) \, \forall s, \forall l \,.$$
<sup>(9)</sup>

This is simply based on the allocation of passenger volume on link *s* to each line in the set of attractive lines ( $l \in \overline{A_s}$ ) by their frequencies.

The other part of the passenger volumes are those using or competing for the service on line l that are associated with other links in the network. Following the structure of the network representation discussed earlier, the service line may also be associated with different links in the network apart from the link under consideration. In this case, we also have to consider the passenger volumes on those links using the same service as the competing flows or contributing flows to the line in-vehicle capacity and congestion respectively, the first term on the right hand-side of Eq. (10) below. In addition, we also have to consider the number of passengers getting on board line *l* at the stop point of link *s* but using a different link in the network, the second term on the right hand-side of Eq. (10) below. These two components of passenger volumes can be combined together, defined as  $\tilde{v}_{sl}$ :

$$\widetilde{v}_{sl} = \sum_{r \in S_{l(s)}^{l+}} v_l^r + \sum_{r \in \overline{S}_{l(s)}^{l}} v_l^r \quad \forall s, \forall l ,$$
(10)

where, i(s) is the origin node of link s,  $S_{i(s)}^{l+}$  indicates the set of links going out from node i(s), but excluding a link s, that contains a line  $l \in \overline{A}^s$  as an attractive line, and  $\overline{S}_{i(s)}^l$  indicates the set of links that contain a line  $l \in \overline{A}^s$  as an attractive line, with origin node before i(s) and end node after i(s).

In matrix form, using the notation introduced earlier, we can define the total passenger volumes competing for or using the capacity of line l over link s as:

$$\mathbf{C} \equiv (\mathbf{\Omega} \mathbf{v}) \otimes \mathbf{A} \tag{11}$$

where **C** is a  $(S \times L+1)$ -matrix with elements  $c_{sl}$  given by:

$$c_{sl} = v_{sl} + \widetilde{v}_{sl} \quad \forall s, \forall l.$$
<sup>(12)</sup>

#### 3.4 Formulation of perceived in-vehicle link travel time

In calculating the perceived in-vehicle travel time, we only need to evaluate the values for the real physical links in the network. These links as included in the hyper-network are the "direct links" defined in the notation section. For the road network and related bus services, the actual travel time is assumed to follow a standard BPR function with an interaction term between the bus and personal vehicle flows. Thus, the actual travel time,  $\bar{t}^s$ , on road link  $s \in S_a$  in the network can be defined as:

$$\bar{t}^{s} = t^{s} \left[ 1 + \beta^{s} \left\{ \left( \sum_{l' \in \psi(s)} f_{l'} E_{b} + V_{pcu}^{s} \right) \middle| K^{s} \right\}^{\gamma^{s}} \right] \forall s \in S_{a},$$
(13)

where,

$$V_{pcu}^{s} = \frac{V^{s}}{O_{a}} E_{a} \quad \forall s \in S_{a},$$
(14)

 $t^s$  and  $K^s$  are the free-flow travel time (in minutes) and capacity (in pcus/hour) of link  $s \in S_a$ respectively;  $\psi(s)$  is a set of bus lines passing through link  $s \in S_a$  in the original network;  $O_a$  is the average occupancy for auto (passengers / auto);  $E_a$  and  $E_b$  are passenger car equivalents for auto and bus respectively; and  $\beta^s$  and  $\gamma^s$  denote calibration parameters.

On the other hand, the actual travel times for underground (or separated transit system) and walking links  $s \in S_u \cup S_w$  are constant, normally given *a priori*. The travel time of bus link  $s \in S_b$  corresponds to the actual travel time of link *s* for auto. As mentioned in the previous section, the effect of travel and in-vehicle congestion is integrated into a single value termed as *perceived travel time*. This will be discussed next.

Define a matrix G as:

$$\mathbf{G} = \begin{bmatrix} \mathbf{C} \otimes \left\{ \mathbf{l} \div (\mathbf{f} \otimes \mathbf{\kappa}) \mathbf{1}_{S}^{T} \right\}^{T} \mid \beta_{1} > 0, \gamma_{1} > 0 \end{bmatrix}$$

$$= \begin{pmatrix} G_{11} & \cdots & G_{1L+1} \\ \vdots & \ddots & \vdots \\ G_{S1} & \cdots & G_{SL+1} \end{pmatrix}$$

$$= \begin{pmatrix} \beta_{1}(g_{11})^{\gamma_{1}} & \cdots & \beta_{1}(g_{1L+1})^{\gamma_{1}} \\ \vdots & \ddots & \vdots \\ \beta_{1}(g_{S1})^{\gamma_{1}} & \cdots & \beta_{1}(g_{SL+1})^{\gamma_{1}} \end{pmatrix},$$
(15)

where the element  $g_{sl}$ , as in Eq.(10), is the  $s^{\text{th}}$  row and  $l^{\text{th}}$  column of  $\mathbf{C} \otimes \{\mathbf{l} \div (\mathbf{f} \otimes \mathbf{\kappa}) \mathbf{1}_{S}^{T}\}^{T}$ , given by:

$$g_{sl} = (v_{sl} + \tilde{v}_{sl}) / (f_l \kappa_l) \,\forall s, \forall l$$
(16)

Next, let us consider the following two matrices defined by Eqs.(17) and (18):

$$\mathbf{Z} = \{ \mathbf{E}^T (\mathbf{G} \otimes \mathbf{J}) \} \otimes \mathbf{H} \,, \tag{17}$$

$$\mathbf{X} \equiv (\mathbf{E}^T \mathbf{J}) \otimes \mathbf{H} \,. \tag{18}$$

Let  $z_{sl}$  denote the element representing the  $s^{th}$  row and  $l^{th}$  column of matrix **Z**, the variable  $z_{sl}$  equals  $G_{s'l'}$  if line l is an attractive line of  $s \in S_b$ , and 0 otherwise. In this regard, any combination of link and line, denoted (s', l'), must simultaneously satisfy the following two conditions:

- i) the actual travel time of link  $s \in S_b$  is affected by the actual travel time of link  $s' \in S_a$ , in this case, actual travel times of link *s* and link *s*' are equal, or actual travel time of link *s* is expressed as a summation of actual travel times of auto links including link *s*'; and
- ii) link *s*' is a direct link regarding line *l*'.

Accordingly,  $z_{sl}$  is an index expressing the in-vehicle congestion effect of an attractive line *l* over link *s*, and links for walking and auto are all equal to 0 by the definitions of the two links. Let  $x_{sl}$  denote the element representing the *s*<sup>th</sup> row and *l*<sup>th</sup> column of matrix **X**, the variable  $x_{sl}$  equals 1 if link  $s \in S_b$  is a direct link regarding line *l*, and 0 otherwise. The ( $S \times L+1$ ) matrix  $\tilde{\mathbf{t}}$  that expresses perceived travel times on line *l* over link *s* is given by:

$$\widetilde{\mathbf{t}} = \left\{ \overline{\mathbf{t}} (\mathbf{X} + \mathbf{Z}) \right\} \otimes \mathbf{A}, \qquad (19)$$

by using a matrix defined by Eq.(20).

$$\bar{\mathbf{t}} = \mathrm{Ediag}(\mathbf{t}^*). \tag{20}$$

The element  $\tilde{t}_l^s$  denoting the *s*<sup>th</sup> row and *l*<sup>th</sup> column of  $\tilde{\mathbf{t}}$ , i.e. perceived travel time on line *l* over link *s*, is given by:

$$\widetilde{t}_{l}^{s} = \left(\sum_{s' \in \theta(s,l)} \overline{t}_{s'}^{s'}\right) (1 + z_{sl})$$

$$= \left(\sum_{s' \in \theta(s,l)} \overline{t}_{s'}^{s'}\right) \left\{ 1 + \beta_{1} \left(\frac{v_{sl} + \widetilde{v}_{sl}}{f_{l}\kappa_{l}}\right)^{\gamma_{1}} \right\} \quad \forall s, \forall l$$
(21)

where  $\beta_1$  and  $\gamma_1$  are calibration parameters on in-vehicle congestion; and  $\theta$  (*s*, *l*) denotes a set of direct links with respect to line *l* that are included in the set of attractive lines  $l \in \overline{A}^s$  over link *s*. Perceived travel time is expressed by the in-vehicle congestion effect, i.e. a discomfort effect on transit represented by assuming a BPR type function multiplied by the actual travel time (Fernandez *et al* 1994; Nielsen 2000). The S-vector that expresses link perceived travel times is:

$$\hat{\mathbf{t}} = \left[ (\tilde{\mathbf{t}} \mathbf{f}) \otimes \{ \mathbf{l} \div (\mathbf{A} \mathbf{f}) \} \right]^T.$$
(22)

Let  $\hat{t}^s$  denote the  $s^{\text{th}}$  element of  $\hat{\mathbf{t}}$ , then  $\hat{t}^s$  is given by:

$$\hat{t}^{s} = \sum_{l \in \overline{A}^{s}} \tilde{t}_{l}^{s} f_{l} / \sum_{l \in \overline{A}^{s}} f_{l} \quad \forall s.$$
(23)

# 3.5 Formulation of the waiting time

The formulations of the waiting times for bus and underground services follow the concept of an in-vehicle perceived travel time in which we have to consider both the number of passengers already on board and those waiting to board at link *s*. The waiting time for passengers waiting to board at link *s* will then be a function of the number of passengers on related service lines boarding before link *s* and remaining in the vehicle after link *s*, and the number of passengers waiting to get on board at link *s* itself. The first term is  $\tilde{V}^s$  as defined earlier, and the second term is simply  $V^s$ . Following De Cea and Fernandez (1993), we define a vector function as:

$$\mathbf{Q}[(\mathbf{C}\mathbf{1}_{L+1}) \otimes \{\mathbf{l} \div (\mathbf{A}\mathrm{diag}(\mathbf{f})\mathbf{\kappa})\} | \beta_2, \gamma_2]$$
  
$$\equiv \left( \mathcal{Q}^1 \quad \cdots \quad \mathcal{Q}^S \right)^T$$
  
$$= \left( \beta_2 \left( q^1 \right)^{\gamma_2} \quad \cdots \quad \beta_2 \left( q^S \right)^{\gamma_2} \right)^T, \qquad (24)$$

where,  $q^s$  denotes the  $s^{\text{th}}$  element of  $\mathbf{Q}[(\mathbf{C1}_{L+1}) \otimes \{\mathbf{l} \div (\mathbf{A}\text{diag}(\mathbf{f})\mathbf{\kappa})\} | \beta_2, \gamma_2]$ , and is given by:

$$q^{s} = \frac{V^{s} + \widetilde{V}^{s}}{\sum_{l \in \overline{A}^{s}} f_{l} \kappa_{l}} \,\,\forall s \,.$$
<sup>(25)</sup>

The *S*-vector of expected waiting times  $\mathbf{w}$  and its element  $w^s$  representing the  $s^{th}$  element of  $\mathbf{w}$  are given respectively by:

$$\mathbf{w} = 60 \otimes \{\mathbf{l} \div (\mathbf{A}\mathbf{f})\} + \mathbf{Q} \text{ (min.)}, \tag{26}$$

$$w^{s} = \frac{60}{\sum_{l \in \overline{A}^{s}} f_{l}} + \beta_{2} \left( \frac{V^{s} + \widetilde{V}^{s}}{\sum_{l \in \overline{A}^{s}} f_{l} \kappa_{l}} \right)^{\gamma_{2}} \forall s , \qquad (27)$$

by assuming  $\alpha$  used in Eq.(1) equals 1. The first term on the right-hand side of Eq.(27) denotes expected waiting time, calculated by assuming a uniform arrival distribution for passengers, and an exponential arrival distribution for transit services with an average interval of  $1/\sum_{l\in\overline{A}^s} f_l$ . Considering links  $s \in S_b \cup S_u$ , passengers have to wait for the next service if the incoming transit service is already full of passengers; the second term on the right hand side of Eq.(27) denotes the waiting time due to the service capacity in such a situation. For the links  $s \in S_a \cup S_w$ ,  $w^s$  is calculated as 0 because of their definitions.

#### 4. Probit-based SUE and Sensitivity Analysis

The demand matrix, i.e.  $\hat{\mathbf{q}}$ , has entries  $\hat{q}_{rs}$ , representing the number of passengers between OD pair *rs*. A vector of link flows, i.e. the numbers of passengers on all links, is  $\mathbf{V}$ , with disutility vector specific to all links  $\mathbf{d}(\mathbf{V})$ , so that  $d^s(\mathbf{V})$  indicates a disutility specific to link  $s \in S$ . The link-intermodal route incidence matrix,  $\Delta^{rs}$  with elements  $\delta_{s,k}^{rs}$  as defined in Eq.(5), denotes the links comprising each route connecting OD pair *rs*. An assignment of passengers to all intermodal routes between OD pair *rs* is denoted by the vector  $\mathbf{q}^{rs}$ , with elements  $q_k^{rs} \ge 0$ , i.e. the number of passengers using  $k^{th}$  intermodal route between OD pair *rs*. An assignment  $\mathbf{q}^{rs}$  is feasible for demand  $\hat{\mathbf{q}}$  if and only if

$$\sum_{k \in K_{rs}} q_k^{rs} = \hat{q}_{rs} \ \forall rs \tag{28}$$

The number of passengers on link *s* is given by:

$$V^{s} = \sum_{rs} \sum_{k \in K_{rs}} q_{k}^{rs} \delta_{s,k}^{rs} \quad \forall s \in S .$$
<sup>(29)</sup>

The disutility of the  $k^{th}$  intermodal route between OD pair *rs* is given by:

$$du_k^{rs}(\mathbf{V}) = \sum_{m \in \{w, a, b, u\}} \alpha^m \zeta_s^{rs} + \sum_{s \in S} d^s(\mathbf{V}) \delta_{s, k}^{rs} \quad \forall k \in K_{rs}, \forall rs .$$
(30)

Passengers are allowed to respond to changes in network variables by changing their intermodal routes. Passengers' responses are assumed to follow the SUE condition.

Let  $\Phi$  be a mapping from  $\mathfrak{R}^{|\mathbf{n}|} \to \mathfrak{R}^{S}$  that gives the vector of feasible link flows (V) calculated subject to some constraints on network variables, say **n**. The optimization problem of network design for a multi-modal network is written as,

$$\min_{\mathbf{V},\mathbf{n}} Z(\mathbf{V},\mathbf{n}) \tag{31}$$
s.t.

$$\mathbf{V} = \mathbf{\Phi}(\mathbf{n}). \tag{32}$$

There are many possible ways to define the mapping  $\Phi$ , e.g. using Wardrop's UE condition, but in this paper we will adopt the concept of probit SUE. Intermodal route choice behaviour is assumed to follow a random utility model. Let the perceived disutility of the *k*-th intermodal route be the random variable  $DU_k$  given by

$$DU_k = du_k + \varepsilon_k \,, \tag{33}$$

where  $du_k = du_k(\mathbf{p}) (= du_k(\mathbf{V} | \mathbf{\Delta}^{rs}))$  is the mean disutility for the *k*-th intermodal route, and the random errors  $(\varepsilon_1, \varepsilon_2, \cdots)$  follow some joint probability density function with zero mean vector. The disutility vector **du** can be also expressed as a function of link flows, **V**, with a given  $\mathbf{\Delta}^{rs}$ , by using the relationship written in Eq.(29).

Given the route disutility vector **du**, we define the probability of passengers travelling between OD pair *rs* choosing the  $k^{\text{th}}$  intermodal route ( $P_k^{rs}(\mathbf{du})$ ) as:

$$P_k^{rs} = \Pr(DU_k^{rs} \le DU_j^{rs} \ \forall j \in K_{rs}, j \neq k)$$
  
=  $\Pr(du_k^{rs} + \varepsilon_k^{rs} \le du_j^{rs} + \varepsilon_j^{rs} \ \forall j \in K_{rs}, j \neq k) \ \forall k \in K_{rs}, \forall rs ,$  (34)

where Pr(.) denotes probability. Adopting a multivariate normal (MVN) distribution for the random error leads to probit-based SUE.

The SUE intermodal route flow assignment and link flow are the solution to the following two equivalent fixed-point problems:

$$\mathbf{q}^{rs} = \hat{q}_{rs} \otimes \mathbf{P}^{rs} \big( \mathbf{d} \mathbf{u}(\mathbf{q}) \big) \quad \forall rs \,, \tag{35}$$

$$\mathbf{V} - \mathbf{p}(\mathbf{d}(\mathbf{V}))\hat{\mathbf{q}} = \mathbf{0}, \tag{36}$$

where,  $\mathbf{P}^{rs}$  denotes the  $K_{rs}$ -vector of route choice probabilities for OD pair rs, and  $\mathbf{p}$  denotes the  $(S \times rs)$ -link choice probabilities matrix, whose  $s^{th}$  row vector  $\mathbf{p}_{rs}$  is given by:

$$\mathbf{p}_{rs} = \mathbf{\Delta}^{rs} \mathbf{P}^{rs} \quad \forall rs \tag{37}$$

We apply a sensitivity analysis method for the purpose of defining the local linear approximation of the Probit SUE link flows  $V^*$  as a function of the design parameters (**n**) around a given vector of link flows and the design parameters (see Clark and Watling 2002; and Connors *et al* 2005 for the detailed formulation). This will then enable us to develop an efficient algorithm for solving the network design problem for multi-modal networks, which will be discussed next.

#### 5. Network Design Problem for Multi-modal Networks

#### 5.1. Frequency Design Problem (FDP)

It is an important question for public transport operators to determine the frequencies of their services. Due to the nature of the public transport service as a public facility, the frequency of a transit system may not be determined based only on its profitability. If all operators cooperate, the optimal frequency for a transit system can be determined to minimize social cost, i.e. total disutility in the multi-modal network considered in this study. A problem to be discussed in this section is the network design problem where the response from passengers to changes in the network variables is assumed to follow the Probit SUE. The first example is a frequency design problem (FDP) for the multi-modal network, which is similar to the one considered in Gao et al. (2004). This problem is structured as follows: letting a vector of network variables  $\mathbf{n}$  be  $\mathbf{f}$  (denoting the frequencies):

$$\min_{\mathbf{f}} Z_{\mathbf{f}}(\mathbf{V}, \mathbf{f}) = \mathbf{d}(\mathbf{V}(\mathbf{f}), \mathbf{f})^T \mathbf{V}(\mathbf{f}) + \theta \mathbf{F}^T \mathbf{f}$$
s.t.
$$\mathbf{V} = \mathbf{\Phi}(\mathbf{n})$$

$$\mathbf{f} > \mathbf{0}$$
(38)

where  $\theta$  is a coefficient converting into disutility the operational cost caused by the frequency setting, and  $\mathbf{F} = (F_1, ..., F_l, ..., F_{L+1})^T$  is the vector of operational costs per frequency increase on the transit lines. In this problem, the mapping  $\Phi$  gives intermodal link flows  $\mathbf{V}(\mathbf{f})$ calculated subject to  $\mathbf{f} \ge \mathbf{1}$ . The objective function, defined in Eq.(38), is the sum of the total disutility experienced by passengers on the multi-modal network plus the disutility converted from costs caused by the frequency setting.

#### 5.2. Anti-freezing Admixture Dispersion Problem (AADP)

The anti-freezing admixture dispersion in the winter season increases the level of service for the road network in cold regions. On the other hand, in addition to the cost involved in using the anti-freezing mixture, its use is detrimental to wildlife near the road network, to the road facilities themselves, to automobiles and so on. In this context, the road administrator has to determine the amount of anti-freezing mixture dispersion (refereed to as AFMD) while considering the trade-off between positive and negative effects from the dispersion (Fig. 2).

#### [INSERT FIGURE 2]

The positive effect from AFMD can be expressed as an increase in road traffic capacity that would otherwise be reduced by the slipperiness of the road surface in winter. The relationship between traffic capacity and the amount of AFMD can be given by:

$$K^{s}(sal^{s} | K_{0}^{s}, K_{n}^{s}, \rho) = -\frac{K_{n}^{s} - K_{0}^{s}}{\rho \, sal^{s} + 1} + K_{n}^{s}, \ \rho > 0 \ \forall s ,$$
(39)

$$\frac{\partial K^s}{\partial sal^s} > 0 \text{ and } \frac{\partial^2 K^s}{\partial sal^{s^2}} < 0 \quad \forall s$$
(40)



Fig. 2. Effects from the dispersion of antifreezing admixture.

where,  $K^{s}(sal^{s}), sal^{s}, K_{0}^{s}$  and  $K_{n}^{s}$  respectively denote the traffic capacity of link *s* when an amount *sal<sup>s</sup>* of AFMD is used (in the winter season), the amount of AFMD on link *s*, traffic capacity of link *s* in the summer season, and traffic capacity of link *s* when no AFMD is used in the winter season.  $\rho$  denotes a calibration parameter (Fig. 3).

#### [INSERT FIGURE 3]

The resulting Anti-freezing Admixture Dispersion Problem (AADP) for a multimodal network is similar to the FDP considered in the previous section, with the aim to minimise the total disutility across all links. Let the design parameters in this case be **sal** (a vector of the amount of AFMD **sal** =  $(sal^1, ..., sal^s, ..., sal^s)^T$ ), we can then formulate the problem as:

$$\min_{sal} Z_{sal}(\mathbf{V}, sal) = \mathbf{d}(\mathbf{V}(sal), sal)^T \mathbf{V}(sal) + \mu \otimes \mathbf{Co}^T sal$$
s.t.
$$\mathbf{V}(sal) = \mathbf{\Phi}(sal)$$
sal  $\ge \mathbf{0}$ 
(41)

where,  $\mu$  and **Co** =  $(Co^1, ..., Co^s, ..., Co^s)^T$  indicate a coefficient of converting deterioration costs, including costs for dispersion works, caused by AFMD to disutility, and the vector of deterioration costs per AFMD increase, respectively. The objective function defined in Eq.(41) is the sum of the total disutilities experienced by passengers on the multi-modal network plus the disutilities (converted from costs) caused by AFMD.

#### 6. Solution Algorithm

One method of solving NDPs, shown by Eqs.(40) and (41), is to adopt the implicit function programming approach (see for example Sumalee *et al* 2005) utilising the Jacobian of the SUE-flows with respect to the design parameters. In this case, at each outer iteration of the optimization algorithm, information is required regarding the value of the objective function Eq.(40) or Eq.(41) and the Jacobian of the objective function, both evaluated at the SUE flows. This indicates that an inner procedure for calculating the Probit based SUE flows has to be made at each outer iteration. Thus, given a vector of network variables ( $\mathbf{n}_k$ ) at



Fig. 3. Link capacity as a function of the amount of anti-freezing admixture dispersion.

iteration *k*, the optimization process re-calculates the SUE flows, evaluates the objective function at new SUE flows, and calculates the Jacobian of the objective function with respect to the network variables. The algorithm then uses this information to determine the predicted optimal network variables ( $\mathbf{n}_{k+1}$ ) for the next iteration. For this type of algorithm, the Jacobian of the objective functions of Eq. (40) and (41) is provided in Appendix A and B respectively.

As mentioned above, the inner procedure should be made for each outer iteration of the optimization algorithm. This fact indicates that application of the implicit programming algorithm directly to NDP may not be efficient, because of the time–consuming, repeated execution of the inner procedure. Thus, we apply the algorithm presented as follows for the purpose of reducing the number of iterations for the inner procedures:

- Step 0: Set one of any feasible vectors of network variables to be an initial solution  $\mathbf{n}_0$ , and set the outer iteration counter k = 0.
- *Step 1*: Calculate a vector of multimodal network flows  $\mathbf{V}_{k}^{*}(\mathbf{n}_{k})$  expressed as the response from passengers to the present vector of network variables  $\mathbf{n}_{k}$ . This can be calculated by applying MSA (Sheffi 1985).
- Step 2: Define the local linear approximation vector of flows  $\tilde{\mathbf{V}}^*(\mathbf{n})$  in the neighbourhood of  $\mathbf{n}_k$  corresponding to the vector of network variables  $\mathbf{n}$ :

 $\widetilde{\mathbf{V}}^*(\mathbf{n}_{k+1}) \approx \mathbf{V}^*(\mathbf{n}_k) - \mathbf{J}_1^{-1} \mathbf{J}_2(\mathbf{n}_{k+1} - \mathbf{n}_k)$ , where  $\mathbf{J}_1$  and  $\mathbf{J}_2$  are the Jacobians of link cost and link choice probability (based on path choice probability) with respect to the design parameters, that are already defined in existing literature (see Clark and Watling 2002).

- Step 3: Solve a sub-problem for the NDP that is obtained by substituting V with  $\tilde{V}^*(\mathbf{n})$  in the objective functions of  $Z_f(V, \mathbf{f})$  in Eq.(40) (or  $Z_{sal}(V, sal)$  in Eq.(41)). This sub-problem can be solved by applying a standard nonlinear optimization algorithm. The solution obtained here will be denoted as  $\mathbf{n}_{k+1}$ .
- Step 4: If  $\max |\mathbf{n}_{k+1} \mathbf{n}_k| < \varepsilon$  then calculation stops, otherwise set k = k+1 and go to Step 1, where  $\varepsilon$  indicates a predetermined, positive, small value.

Note that the key difference between this and the implicit programming approach is that in Step 3 the information about the sensitivity of the SUE link flows with respect to the design parameters is utilised in formulating local linear approximations of the SUE link flows. The Probit SUE condition as a constraint in the original problem will then be substituted by these linear equality equations. This sub-optimisation problem will then be solved and the updated local linear approximation of the SUE link flows for the next sub-problem will be carried out at the solution of the current sub-problem. This algorithm will be adopted to solve the problems defined in Eq. (40) and (41) in the next section.

#### 7. Numerical Experiments

#### 7.1. Definition of the Test Network

A primitive network and its hyper-network adopted for the test are shown in Fig. 4. The network shown in Fig. 4a is a primitive network and has 4 transit lines, 6 road links and 4 walking links. Line 1 indicates a subway line whose itinerary is  $x \rightarrow z$ . Line 2, Line 3 and Line 4 indicate bus lines whose itineraries are  $w \rightarrow x \rightarrow y$ ,  $w \rightarrow x \rightarrow z$  and  $x \rightarrow y \rightarrow z$ , respectively. The hyper-network shown in Fig. 4b has 11 nodes and 18 links. Links in the hyper-network are developed by distinguishing between the two transit systems, i.e. subway system and bus system, because of the complication of the preference evaluation (Nielsen 2000) and the differences in characteristics between the systems. For simplicity, all lines are assumed to be attractive lines.

#### [INSERT FIGURE 4]

There are two OD movements, i.e. from node  $O_1$  to node  $D_1$  and from node  $O_2$  to node  $D_2$ , and the numbers of passengers for the two OD movements are 5000 and 1000 (passengers/hr), respectively. The passengers between OD pair  $O_1D_1$  can use all transport modes whereas the passengers between OD pair  $O_2D_2$  can use only the bus system. Table 1



(b) The test hyper network.

Fig. 4. Network representations for the multi-modal network.

and Table 2 show the coefficients of link disutility and the coefficients of line disutility, respectively.  $O_a, E_a$  and  $E_b$  defined in Eqs.(19) and (20) are all set as 1.0.

#### [INSERT TABLE 1]

#### [INSERT TABLE 2]

A random error term (with zero mean and standard deviation  $\sigma_{s_m}$ ) is defined for each link  $s_m \in S$ . A the standard deviation of the random error term for each link is set as 30% of that link's free flow disutility without the monetary term. The variance-covariance matrix, for a MVN distribution, with respect to disutilities for intermodal routes is created from the linkpath incidence matrix, and these predefined variances of the error terms associated independently with each of the links in the network.

#### 7.2. Results for Frequency Design Problem

Fig. 5 shows the modal shares of the passengers between OD pair  $O_1D_1$  when the frequencies of transit lines of 1 and 3 vary, i.e. the subway line and bus line respectively, where frequencies of line 2 and line 4 are fixed at 5 (services/hour). The modal share of subway increases as the subway line frequency increases, i.e. changing from about 5% at a subway frequency of 1 services/hour, to 50% at a subway frequency of 20 services/hour.

#### [INSERT FIGURE 5]

Similarly, the modal share of auto decreases as the subway line frequency increases, changing from about 80% to 30%. As the subway line frequency changes, for  $O_1D_1$  most transport mode switching occurs between the subway and auto, with only a small change to the bus's share.

On the other hand, as the frequency of the bus line is increased, the modal share of bus increases slightly and there is a small change to the share for auto and subway. The bus network is heavily occupied by the passengers between OD pair  $O_2D_2$ , who can only use the bus system. This is the reason for the insensitivity to the bus frequency of the bus share between OD pair  $O_1D_1$ .

# TABLE 1

Coefficients of link disutility

link	link mode fa		free travel time: $t^s$ (min)	road capacity: K <sup>sa</sup> (pcu/hr)	parameters for auto: $\beta^{sa}$ , $\gamma^{sa}$
1	sub	200	10		
2	bus	190	15		
3	bus	150	5		
4	bus	170	10		
5	bus	150	5		
6	bus	170	10		
7	bus	150	5		
8	auto		5	1000	1, 2
9	auto		5	1000	1, 2
10	auto		5	1000	1, 2
11	auto		5	1000	1, 2
12	auto		5	1000	1, 2
13	auto		5	1000	1, 2
14	walk		3		
15	walk		3		
16	walk		3		
17	walk		3		
18	walk		3		

TABLE 2Coefficients of line disutility

		vehicle capacity	mode	coefficients	parameters for	parameters for				
line	mode	$(\kappa_l)$	specific	for link	waiting time	discomfort				
	moue	(passengers/service)	constants	disutility	function ( $\beta_2, \gamma_2$ )	function				
			$(\alpha^m)$	$(\pi^m, \rho^m, \tau^m)$		$(\beta_1, \gamma_1)$				
1	sub	100	10	1, 1, 0.02	2, 3	2, 3				
2	bus	50	20	1, 1, 0.02	2, 3	2, 3				
3	bus	50	20	1, 1, 0.02	2, 3	2, 3				
4	bus	50	20	1, 1, 0.02	2, 3	2, 3				
5	auto	00	50	1, 1, 0.02						
6	walk	00	5	1, 1, 0.02						



Fig. 5. Modal shares of passengers between  $O_1D_1$  for the FDP.

In the case of the subway, the increase in the frequency of the subway service can decrease the disutility of the subway system dramatically. Both the expected waiting time and the in-vehicle discomfort decrease, so that passengers change transport mode from auto to subway. Thus, the modal share of subway is relatively sensitive to the frequency changes of the subway. This is different from the situation with the bus system.

Next, we consider the FDP for the transit lines. Fig. 6 shows the surface of the objective function as the frequencies of transit lines 1 and 3 vary (with fixed frequencies on transit lines 2 and 4, of 5 services/hour). The fares per frequency increase ( $F_l$ ) on transit line l (=1,...,4) are set as 50, 20, 40 and 20, respectively. From Fig. 6, the objective function suggested an optimal solution of the frequencies for transit lines 1 and 3 are not at the boundary (i.e. interior solution).

#### **[INSERT FIGURE 6]**

With a lower level of frequencies for the transit lines, the expected waiting time and in-vehicle discomfort increase, so does the total disutility in the network. In the case of a high level of frequencies of the transit lines, both the expected waiting time and in-vehicle discomfort decrease, while the disutility converted fare caused by frequency setting increases. As a result, the total disutility in the multi-modal network increases as a whole. In general, judging from these facts, an optimal solution of the FDP should be an interior solution (as shown in Figure 6).

We applied the algorithm mentioned above to solve the optimal frequencies of the transit lines problem. Fig. 7 shows the contours of the objective function (as shown in Fig. 6) with the trajectory of the optimization process of  $f_1$  and  $f_3$  starting from a set of initial solutions of  $(f_1, f_3) = (1.00, 1.00)$ . The optimal solution and the value of optimized objective function found during the third outer iteration of the algorithm are  $(f_1^*, f_3^*) = (14.85, 11.66)$  and  $2.2697 \times 10^6$  respectively. The modal shares of subway, bus and auto by the passengers between OD pair  $O_1D_1$ , at optimal frequencies of line 1 and line 3, are 50%, 5% and 45%,



Fig. 6. Surface of the objective function for the FDP.

respectively. The algorithm also obtained the same solutions even when we started the optimization process from different initial solutions.

#### [INSERT FIGURE 7]

The solutions, obtained in the case when all frequencies of four transit lines are optimized, are  $(f_1^*, f_2^*, f_3^*, f_4^*) = (12.57, 16.37, 1.00, 20.11)$ , and the value of the objective function at optimal frequencies is  $2.2295 \times 10^6$ . The modal shares of subway, bus and auto by the passengers between OD pair O<sub>1</sub>D<sub>1</sub>, at optimal frequencies of all lines, are 47%, 10% and 43%, respectively. Note that the optimal frequency of line 3 is calculated as 1.0, which is the minimum value determined by the constraints. This implies that it is not worthwhile (against the cost of improvement) to improve the frequency of line 3 to reduce the total disutility in the multimodal network. In this context, it is better that line 3 is eliminated. The problem dealt with here, i.e. FDP, can give one possible standard for judging transit's efficiency in terms of disutility that does not depend on profitability.

#### 7.3. Results for the Anti-freezing Admixture Dispersion Problem

Fig. 8 shows changes in modal shares for the passengers between OD pair  $O_1D_1$  both in summer and in winter, based on the assumption that traffic capacities in winter decrease from those in summer, where a vector of transit frequencies is set as  $\mathbf{f} = (5, 10, 10, 10, \infty)^T$ . The calibration parameter  $\rho$  in Eq.(46) is set equal to 1. From Fig. 8, there are large numbers of passengers who change transport mode depending on the season, especially the change from auto in summer to subway in winter.

### [INSERT FIGURE 8]

Fig. 9 shows modal shares of the passengers between OD pair  $O_1D_1$  when the amount of AFMD on links 9 and 10 vary, while the amount of AFMD on the other links is fixed at 0. Using AFMD on these two links brings about changes in transport mode between auto and bus; on the other hand, the modal share of subway does not show any big differences.

#### [INSERT FIGURE 9]



Fig. 7. Contours of the objective function and trajectory of the optimization process for the FDP.



Fig. 8. Modal shares of passengers between O<sub>1</sub>D<sub>1</sub> in summer and winter seasons.



Fig. 9. Modal shares of passengers between  $O_1D_1$  for the AADP.

Fig. 10 shows the surface of the objective function as the amounts of AFMD on links 9 and 10 vary (with the amount of anti-freezing admixture dispersed on the other links fixed at 0). The vector of deterioration costs per AFMD increase is set as  $\mathbf{Co}^{8\sim13} = (800, 200, 800, 1000, 1000)^T$ . From Fig. 10, the objective function seems to be more sensitive to the amount of AFMD on link 9 than the amount on link 10.

#### [INSERT FIGURE 10]

Fig. 11 shows the contours of the objective function (as shown in Fig. 10) with the trajectory of the optimization process of  $sal^9$  and  $sal^{10}$  starting from a set of initial solutions of  $(sal^9, sal^{10}) = (0.00, 0.00)$ . The optimal solution and the optimal value of the objective function found during the third outer iteration of the algorithm are  $(sal^{9^*}, sal^{10^*}) = (3.97, 2.06)$  and  $1.3852 \times 10^5$  respectively. The modal shares of subway, bus and auto by the passengers between OD pair O<sub>1</sub>D<sub>1</sub>, at optimal dispersions of link 9 and link 10, are 58.4%, 20.3% and 21.4%, respectively. The algorithm also obtained the same solutions when we started the optimization process from different initial conditions. The differences in the optimal amounts of AFMD on links 9 and 10 come from their deterioration costs per AFMD increase. When the optimal dispersions are made in the winter season, the ratios of capacities for links 9 and 10 correspond to 90% and 84% of those in summer season, respectively.

#### [INSERT FIGURE 11]

The solutions, obtained in the case where amounts of dispersion on all road links are optimized, are  $sal^{8-13} = (1.92, 5.06, 2.49, 0.53, 0.85, 0.53)^T$ , and the value of the objective function at optimal dispersions is  $1.3540 \times 10^5$ . The amount of dispersion on link 8 is much less than that on link 10 despite their same deterioration costs per a unit of AFMD, and despite the fact that link 8 is used by all passengers between OD pair  $O_1D_1$  who choose auto. This is because of the different effects from bus lines, i.e. dispersion on link 8 cannot reduce disutilities for the passengers who choose bus, whereas dispersion on link 10 can do this. The ratios of capacities for links from 8 to 13 when the optimal dispersions are made in winter



Fig. 10. Surface of objective function for the AADP.



Fig. 11. Contours of the objective function and trajectory of the optimization process for the AADP.

season correspond to 82.8%, 91.7%, 85.7%, 67.3%, 73.0% and 67.3% of those in summer season, respectively. The modal shares of subway, bus and auto by the passengers between OD pair  $O_1D_1$ , at optimal dispersions, are 57.0%, 21.7% and 21.3%, respectively.

#### 8. Concluding Remarks

In this study, a probit-based multi-modal transport assignment model is proposed. Three transport modes—railway system, bus system and auto—are considered simultaneously in the model, allowing for the interaction effect of the congestion caused by autos and buses. Two network design problems, the FDP and AADP, are formulated as implicit programs in which the objective functions are to minimize total disutility in the multi-modal network at the SUE flows, by changing the network variables. Two numerical examples are given to illustrate the model and algorithm proposed. It is found, based on some tests that the algorithm finds the same optimal solution regardless of the initial conditions given. However, the uniqueness of the solution may strongly depend on the coefficients of the disutility functions, since these coefficients influence the uniqueness of the probit-based SUE flows for a multi-modal traffic assignment with asymmetric link disutility functions. Further examination of the uniqueness and stability of the multi-modal traffic assignment model proposed in this study is required. This research topic will be addressed in a future study.

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#### References

- Abdulaal, M. & LeBlanc, L.J. (1979) Continuous equilibrium network design models, *Transportation Research Part B* 13 (1), 19-32.
- Chiriqui, C. & Robillard, P. (1975) Common bus lines, Transportation Science 9, 115-21.
- Clark, S.D. & Watling, D.P. (2002) Sensitivity analysis of the probit-based stochastic user equilibrium assignment model, *Transportation Research Part B* 36 (7), 617-35.
- Connors, R.D., Sumalee, A. & Watling, D.P. (2005) Sensitivity Analysis of the Variable Demand Probit Stochastic User Equilibrium with Multiple User-Classes, *Transportation Research Part B* submitted.
- De Cea, J. & Fernandez, E. (1993) Transit assignment for congested public transport system: An equilibrium model, *Transportation Science* 27, 133-47.
- Fernandez, E., De Cea, J., Florian, M. & Cabrera, E. (1994) Network equilibrium models with combined modes, *Transportation Science* 28, 182-92.
- Gao, Z.Y., Sun, H. & Shan, L.L. (2004) A continuous equilibrium network design model and algorithm for transit systems, *Transportation Research Part B* 38 (3), 235-50.
- Kraus, M. (1991) Discomfort Externalities and Marginal Cost Transit Fares, *Journal of Urban Economics* 29, 249-59.
- Kurauchi, F., Schomoecker, J.-D. & Bell, M.G.H. (2003) Capacity Constrained Transit Assignment with Common Lines, *Journal of Mathematical Modelling and Algorithms* 2, 309-27.
- Lam, W.H.K., Gao, Z.Y., Chan, K.S. & Yang, H. (1999) A stochastic user equilibrium assignment model for congested transit networks, *Transportation Research Part B* 33 (5), 351-68.
- Lawphongpanich, S. & Hearn, D.W. (2004) An MPEC Approach to Second-Best Toll Pricing, *Mathematical Programming B* 101 (1), 33-55.
- Lo, H.K., Yip, C.W. & Wan, K.H. (2003) Modelling transfer and non-linear fare structure in multi-modal network, *Transportation Research Part B* 37 (2), 149-70.
- Nielsen, O.A. (2000) A stochastic transit assignment model considering difference in passenger utility functions, *Transportation Research Part B* 34 (5), 377-402.
- Shepherd, S.P. & Sumalee, A. (2004) A Genetic Algorithm Based Approach to Optimal Toll Level and Location Problems, *Networks and Spatial Economics* 4, 161-79.
- Spiess, H. 1983, *On optimal route choice strategies in transit networks*, Pub. 286, Centre de Recherche sur les Transports, University of Montreal.
- Spiess, H. & Florian, M. (1989) Optimal strategies: A new assignment model for transit network, *Transportation Research Part B* 23 (2), 83-102.
- Sumalee, A., Connors, R. & Watling, D.P. (2005) Optimal toll design problem with improved behavioural equilibrium model: the case of Probit model. *Mathematical and Computational Models for Congestion Charging*, eds DW Hearn, S Lawphongpanich & MJ Smith, Springer, Berlin, Germany.
- Tobin, R.L. & Friesz, T.L. (1988) Sensitivity Analysis for Equilibrium Network Flow, *Transportation Science* 22 (4), 242-50.
- Yang, H. & Bell, M.G.H. (1997) Traffic restraint, road pricing and network equilibrium, *Transportation Research Part B* 31 (4), 303-14.

# Appendix A. Jacobians for frequency design problem

The ( $S \times 1$ )-Jacobian vector of the objective function given by Eq.(44) with respect to frequency vector **f** is:

$$\frac{\partial Z_{\mathbf{f}}}{\partial \mathbf{f}} = \left(\frac{\partial \mathbf{d}}{\partial \mathbf{f}}\right)^{T} \mathbf{V}^{*} + \left(\frac{\partial \mathbf{V}^{*}}{\partial \mathbf{f}}\right)^{T} \mathbf{d} + \boldsymbol{\theta} \otimes \mathbf{F}$$
$$= \left\{ \left(\frac{\partial \mathbf{d}}{\partial \mathbf{f}}\right)^{T} + \left(\frac{\partial \mathbf{V}^{*}}{\partial \mathbf{f}}\right)^{T} \left(\frac{\partial \mathbf{d}}{\partial \mathbf{V}^{*}}\right) \right\} \mathbf{V}^{*} + \left(\frac{\partial \mathbf{V}^{*}}{\partial \mathbf{f}}\right)^{T} \mathbf{d} + \boldsymbol{\theta} \otimes \mathbf{F}, \qquad (A.1)$$

where

$$\frac{\partial \mathbf{d}}{\partial \mathbf{f}} = \boldsymbol{\pi} \otimes \frac{\partial \hat{\mathbf{t}}}{\partial \mathbf{f}} + \boldsymbol{\rho} \otimes \frac{\partial \mathbf{w}}{\partial \mathbf{f}}, \qquad (A.2)$$

$$\frac{\partial \mathbf{d}}{\partial \mathbf{V}} = \boldsymbol{\pi} \otimes \frac{\partial \hat{\mathbf{t}}}{\partial \mathbf{V}} + \boldsymbol{\rho} \otimes \frac{\partial \mathbf{w}}{\partial \mathbf{V}}.$$
(A.3)

 $\partial \hat{\mathbf{t}} / \partial \mathbf{f}$  in Eq.(A.2) is a ( $S \times L + 1$ )-matrix, and the  $l^{\text{th}}$  row vector of the matrix is given

by:

$$\frac{\partial \hat{\mathbf{t}}}{\partial f_l} = \left(\frac{\partial \tilde{\mathbf{t}}}{\partial f_l} \mathbf{f} + \tilde{\mathbf{t}} \frac{\partial \mathbf{f}}{\partial f_l}\right) \otimes \{\mathbf{l} \div (\mathbf{A}\mathbf{f})\} + (\tilde{\mathbf{t}}\mathbf{f}) \otimes \frac{\partial \{\mathbf{l} \div (\mathbf{A}\mathbf{f})\}}{\partial f_l} \text{ if } l \neq L + 1,$$
$$\frac{\partial \hat{\mathbf{t}}}{\partial f_l} = \mathbf{0} \quad \text{otherwise,} \tag{A.4}$$

where the following two relationships hold.

$$\frac{\partial \tilde{\mathbf{t}}}{\partial f_l} = \left\{ \frac{\partial \bar{\mathbf{t}}}{\partial f_l} (\mathbf{Z} + \mathbf{X}) \right\} \otimes \mathbf{A} + \left( \bar{\mathbf{t}} \frac{\partial \mathbf{Z}}{\partial f_l} \right) \otimes \mathbf{A} , \qquad (A.5)$$

$$\frac{\partial \{\mathbf{l} \div (\mathbf{A}\mathbf{f})\}}{\partial f_l} = \mathbf{A}(:,l) \otimes \left[-1 \div \{(\mathbf{A}\mathbf{f}) \otimes (\mathbf{A}\mathbf{f})\}\right].$$
(A.6)

A(:, *l*) in Eq.(A.5) is a vector indicating the  $l^{\text{th}}$  row of matrix A. (L + 1)-vector of  $\partial \mathbf{f} / \partial f_l$  in (A.4) has  $l^{\text{th}}$  element of 1, and 0 otherwise.  $\partial \bar{\mathbf{t}} / \partial f_l$  in Eq.(A.5) is given by:

$$\frac{\partial \bar{\mathbf{t}}}{\partial f_l} = \mathbf{E} \frac{\partial \left\{ \operatorname{diag}(\mathbf{t}^*) \right\}}{\partial f_l}, \qquad (A.7)$$

where  $\partial \{ \operatorname{diag}(\mathbf{t}^*) \} / \partial f_l$  in Eq.(A.7) is a  $(S \times L + 1)$ -matrix, and  $s^{\text{th}}$  row and  $l^{\text{th}}$  column of the matrix is:

$$\frac{\partial \bar{t}^s}{\partial f_l} = h_{sl} t^s \beta^s \gamma^s \left(\frac{E_b}{K^s}\right) \left(\frac{V_{pcu}^s}{K^s}\right)^{\gamma^s - 1} \text{ if } l \neq L + 1,$$

$$\frac{\partial \bar{t}^s}{\partial f_l} = 0 \text{ otherwise.}$$
(A.8)

 $\partial \mathbf{Z} / \partial f_l$  in Eq.(A.5) is given by:

$$\frac{\partial \mathbf{Z}}{\partial f_l} = \left\{ \mathbf{E}^T \left( \frac{\partial \mathbf{G}}{\partial f_l} \otimes \mathbf{J} \right) \right\} \otimes \mathbf{H} , \qquad (A.9)$$

where the following relationship holds.

$$\frac{\partial \mathbf{G}}{\partial f_l} = \mathbf{G} \left[ \mathbf{C} \otimes \left\{ \mathbf{l} \div (\mathbf{f} \otimes \mathbf{\kappa}) \mathbf{1}_S^T \right\}^T | \beta_1 \gamma_1, \gamma_1 - 1 \right]$$
$$\otimes \left[ \frac{\partial \mathbf{C}}{\partial f_l} \otimes \left\{ \mathbf{l} \div (\mathbf{f} \otimes \mathbf{\kappa}) \mathbf{1}_S^T \right\}^T + \mathbf{C} \otimes \frac{\partial \left\{ \mathbf{l} \div (\mathbf{f} \otimes \mathbf{\kappa}) \mathbf{1}_S^T \right\}^T}{\partial f_l} \right].$$
(A.10)

 $\partial \mathbf{C} / \partial f_l$  in Eq.(A.10) is given by:

$$\frac{\partial \mathbf{C}}{\partial f_l} = \left\langle \mathbf{\Omega} \left[ \left\{ \mathbf{A} \operatorname{diag} \left( \frac{\partial \mathbf{f}}{\partial f_l} \right) \right\} \otimes \left( \mathbf{P} \mathbf{1}_{L+1}^T \right) + \left\{ \mathbf{A} \operatorname{diag} (\mathbf{f}) \right\} \otimes \left( \frac{\partial \mathbf{P}}{\partial f_l} \mathbf{1}_{L+1}^T \right) \right] \right\rangle \otimes \mathbf{A} , \qquad (A.11)$$

where the following relationship holds.

$$\frac{\partial \mathbf{P}}{\partial f_l} = \mathbf{V} \otimes \frac{\partial \{\mathbf{l} \div (\mathbf{A}\mathbf{f})\}}{\partial f_l} \,. \tag{A.12}$$

 $\partial \left\{ \mathbf{l} \div (\mathbf{f} \otimes \mathbf{\kappa}) \mathbf{l}_{S}^{T} \right\}^{T} / \partial f_{l}$  in Eq.(A.10) is given by:

$$\frac{\partial \left\{ \mathbf{l} \div (\mathbf{f} \otimes \mathbf{\kappa}) \mathbf{l}_{S}^{T} \right\}^{T}}{\partial f_{l}} = \mathbf{A}_{l} \otimes \left\langle -1 \div \left\{ (\mathbf{\kappa} \otimes \mathbf{f} \otimes \mathbf{f}) \mathbf{l}_{S}^{T} \right\}^{T} \right\rangle, \tag{A.13}$$

where  $\mathbf{A}_l$  in Eq(A.13) is a  $(S \times L + 1)$ -matrix and  $l^{\text{th}}$  row of the matrix is  $\mathbf{A}(:, l)$  and  $\mathbf{0}$  otherwise.

 $\partial \hat{\mathbf{t}} / \partial \mathbf{V}$  in Eq.(A.2) is a (S × S)-matrix and s<sup>th</sup> row of the matrix is given by:

$$\frac{\partial \hat{\mathbf{t}}}{\partial V^s} = \left(\frac{\partial \tilde{\mathbf{t}}}{\partial V^s} \mathbf{f}\right) \otimes \{\mathbf{l} \div (\mathbf{A}\mathbf{f})\},\tag{A.14}$$

where the following relationship holds.

$$\frac{\partial \tilde{\mathbf{t}}}{\partial V^s} = \left\{ \frac{\partial \bar{\mathbf{t}}}{\partial V^s} (\mathbf{Z} + \mathbf{X}) + \bar{\mathbf{t}} \frac{\partial \mathbf{Z}}{\partial V^s} \right\} \otimes \mathbf{A} .$$
(A.15)

 $\partial \bar{\mathbf{t}} / \partial V^s$  in Eq.(A.15) is:

$$\frac{\partial \bar{\mathbf{t}}}{\partial V^s} = \mathbf{E} \frac{\partial \{ \operatorname{diag}(\mathbf{t}^*) \}}{\partial V^s}, \qquad (A.16)$$

where  $\partial \{ \operatorname{diag}(\mathbf{t}^*) \} / \partial V^s$  in Eq.(A.16) is a ( $S \times S$ )-matrix, and  $s^{\text{th}}$  row and  $s^{\text{th}}$  column of the matrix is given by:

$$\frac{\partial \bar{t}^s}{\partial V^{s'}} = \begin{cases} t^s \beta^s \gamma^s \left(\frac{E_a}{O_a}\right) \left(\frac{V_{pcu}^s}{K^s}\right)^{\gamma^s - 1} & \text{if } s \in S_a \text{ and } s = s', \\ 0 & \text{otherwise.} \end{cases}$$
(A.17)

 $\partial \mathbf{Z} / \partial V^s$  in Eq.(A.15) is given by:

$$\frac{\partial \mathbf{Z}}{\partial V^s} = \left\{ \mathbf{E}^T \left( \frac{\partial \mathbf{G}}{\partial V^s} \otimes \mathbf{J} \right) \right\} \otimes \mathbf{H} , \qquad (A.18)$$

where the following relationship holds.

$$\frac{\partial \mathbf{G}}{\partial V^s} = \mathbf{G} \left[ \mathbf{C} \otimes \left\{ \mathbf{l} \div (\mathbf{f} \otimes \mathbf{\kappa}) \mathbf{1}_s^T \right\}^T | \beta_1 \gamma_1, \gamma_1 - 1 \right] \otimes \left\langle \frac{\partial \mathbf{C}}{\partial V^s} \otimes \left[ \left\{ \mathbf{l} \div (\mathbf{f} \otimes \mathbf{\kappa}) \mathbf{1}_s^T \right\}^T \right] \right\rangle. (A.19)$$

 $\partial \mathbf{C} / \partial V^s$  in Eq.(A.19) is given by:

$$\frac{\partial \mathbf{C}}{\partial V^s} = \left[ \mathbf{\Omega} \left\{ \left( \mathbf{A} \operatorname{diag}(\mathbf{f}) \right) \otimes \left( \frac{\partial \mathbf{P}}{\partial V^s} \mathbf{1}_{L+1}^T \right) \right\} \right] \otimes \mathbf{A}, \qquad (A.20)$$

where the following relationship holds.

$$\frac{\partial \mathbf{P}}{\partial V^s} = \frac{\partial \mathbf{V}}{\partial V^s} \otimes \left\{ \mathbf{l} \div (\mathbf{A}\mathbf{f}) \right\}.$$
(A.21)

 $\partial \mathbf{V} / \partial V^s$  in Eq.(A.21) is a S-vector and  $s^{\text{th}}$  element of the vector is 1 and 0 otherwise.

 $\partial \mathbf{w} / \partial \mathbf{f}$  in Eq.(A.2) is a ( $S \times L + 1$ )-matrix and  $l^{\text{th}}$  row of the matrix is:

$$\frac{\partial \mathbf{w}}{\partial f_l} = 60 \otimes \frac{\partial \{\mathbf{l} \div (\mathbf{AF})\}}{\partial f_l} + \frac{\partial \mathbf{Q}}{\partial f_l} \text{ if } l \neq L + 1,$$

$$\frac{\partial \mathbf{w}}{\partial f_l} = \mathbf{0} \text{ otherwise,} \tag{A.22}$$

where the following relationship holds.

$$\frac{\partial \mathbf{Q}}{\partial f_{l}} = \mathbf{Q} [(\mathbf{C}\mathbf{1}_{L+1}) \otimes \{\mathbf{l} \div (\mathbf{A} \operatorname{diag}(\mathbf{f})\mathbf{\kappa})\} | \beta_{2}\gamma_{2}, \gamma_{2} - \mathbf{l}] \\ \otimes \left[ \left( \frac{\partial \mathbf{C}}{\partial f_{l}} \mathbf{1}_{L+1} \right) \otimes \{\mathbf{l} \div (\mathbf{A} \operatorname{diag}(\mathbf{f})\mathbf{\kappa})\} + (\mathbf{C}\mathbf{1}_{L+1}) \otimes \frac{\partial \{\mathbf{l} \div (\mathbf{A} \operatorname{diag}(\mathbf{f})\mathbf{\kappa})\}}{\partial f_{l}} \right].$$
(A.23)

 $\partial \{ l \div (A \operatorname{diag}(\mathbf{f}) \kappa) \} / \partial f_l \text{ in Eq.}(A.23) \text{ is given by:}$ 

$$\frac{\partial \{\mathbf{l} \div (\mathbf{A} \operatorname{diag}(\mathbf{f}) \mathbf{\kappa})\}}{\partial f_l} = \mathbf{A}(:,l) \otimes \left[-\kappa_l \div \{(\mathbf{A} \operatorname{diag}(\mathbf{f}) \mathbf{\kappa}) \otimes (\mathbf{A} \operatorname{diag}(\mathbf{f}) \mathbf{\kappa})\}\right].$$
(A.24)

 $\partial \mathbf{w} / \partial \mathbf{V}$  in (A.2) is a (*S* × *S*) matrix and *s*<sup>th</sup> row of the matrix is:

$$\frac{\partial \mathbf{w}}{\partial V^{s}} = \frac{\partial \mathbf{Q}}{\partial V^{s}}$$
$$= \mathbf{Q} [(\mathbf{C} \mathbf{1}_{L+1}) \otimes \{\mathbf{l} \div (\mathbf{A} \operatorname{diag}(\mathbf{f}) \mathbf{\kappa})\} | \beta_{2} \gamma_{2}, \gamma_{2} - 1]$$
$$\otimes \left[ \left( \frac{\partial \mathbf{C}}{\partial V^{s}} \mathbf{1}_{L+1} \right) \otimes \{\mathbf{l} \div (\mathbf{A} \operatorname{diag}(\mathbf{f}) \mathbf{\kappa})\} \right].$$
(A.25)

#### Appendix B. Jacobians for anti-freezing admixture dispersion problem

# The $(S \times 1)$ -Jacobian vector of the objective function expressed by Eq.(48) with

respect to amounts of anti-freezing admixture dispersions vector sal is:

$$\frac{\partial Z_{\text{sal}}}{\partial \text{sal}} = \left(\frac{\partial \mathbf{d}}{\partial \text{sal}}\right)^T \mathbf{V}^* + \left(\frac{\partial \mathbf{V}^*}{\partial \text{sal}}\right)^T \mathbf{d} + \mu \otimes \mathbf{Co}$$

$$= \left\{ \left(\frac{\partial \mathbf{d}}{\partial \text{sal}}\right)^T + \left(\frac{\partial \mathbf{V}^*}{\partial \text{sal}}\right)^T \left(\frac{\partial \mathbf{d}}{\partial \mathbf{V}^*}\right) \right\} \mathbf{V}^* + \left(\frac{\partial \mathbf{V}^*}{\partial \text{sal}}\right)^T \mathbf{d} + \mu \otimes \mathbf{Co}$$
(B.1)

where,

$$\frac{\partial \mathbf{d}}{\partial \mathbf{sal}} = \boldsymbol{\pi} \otimes \frac{\partial \hat{\mathbf{t}}}{\partial \mathbf{sal}},\tag{B.2}$$

$$\frac{\partial \mathbf{d}}{\partial \mathbf{V}} = \boldsymbol{\pi} \otimes \frac{\partial \hat{\mathbf{t}}}{\partial \mathbf{V}} + \boldsymbol{\rho} \otimes \frac{\partial \mathbf{w}}{\partial \mathbf{V}} \,. \tag{B.3}$$

Because Eq.(B.3) has the same form as explained in Appendix A, we only need consider Eq.(B.2).  $\partial \hat{\mathbf{t}} / \partial \mathbf{sal}$  in Eq.(B.2) is a ( $S \times S$ ) matrix and  $s^{\text{th}}$  row of the matrix is given by:

$$\frac{\partial \hat{\mathbf{t}}}{\partial sal^s} = \left[ \left( \frac{\partial \tilde{\mathbf{t}}}{\partial sal^s} \mathbf{f} \right) \otimes \left\{ 1 \div (\mathbf{A}\mathbf{f}) \right\} \right]^T, \tag{B.3}$$

where the following two relationships hold.

$$\frac{\partial \tilde{\mathbf{t}}}{\partial sal^s} = \left\{ \frac{\partial \bar{\mathbf{t}}}{\partial sal^s} (\mathbf{Z} + \mathbf{X}) \right\} \otimes \mathbf{A} , \qquad (B.4)$$

$$\frac{\partial \bar{\mathbf{t}}}{\partial sal^s} = \operatorname{Ediag}\left(\frac{\partial \mathbf{t}^*}{\partial sal^s}\right). \tag{B.5}$$

 $\partial t^* / \partial sal^s$  in Eq.(B.4) is a (S×1) vector and its s<sup>th</sup> element ( $\partial t^{*s} / \partial sal^s$ ) of the vector is:

$$\frac{\partial t^{*s}}{\partial sal^{s}} = -t^{s} \alpha^{s} \beta^{s} V_{pcu}^{s} K^{s} (sal^{s})^{-(\beta^{s}+1)} \cdot \frac{K_{n}^{s} - K_{0}^{s}}{(\rho \cdot sal^{s}+1)^{2}} \text{ if } s \in S_{a}, \frac{\partial t^{*s}}{\partial sal^{s}} = 0 \text{ otherwise.}$$
(B.6)