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A predictive continuum dynamic user-optimal model for the simultaneous departure time and route choice problem in a polycentric city

#### Zhi-Yang Lin

Shanghai Institute of Applied Mathematics and Mechanics, Shanghai University, Shanghai, China, linzy\_1990@shu.edu.cn

S. C. Wong

Department of Civil Engineering, The University of Hong Kong, Pokfulam Road, Hong Kong, hhecwsc@hku.hk

#### Peng Zhang

Shanghai Institute of Applied Mathematics and Mechanics, Shanghai University, Shanghai, China Shanghai Key Laboratory of Mechanics in Energy Engineering, pzhang@mail.shu.edu.cn

#### Keechoo Choi

Department of Transportation Engineering, TOD-based Sustainable Urban Transportation Center, Ajou University, Republic of Korea, keechoo@ajou.ac.kr

This study develops a predictive continuum dynamic user-optimal model for the simultaneous departure time and route choice problem through a variational inequality (VI) approach. A polycentric urban city with multiple central business districts (CBDs) is considered, and travelers are classified into different classes according to their destinations (i.e., CBDs). The road network within the modeling city is assumed to be sufficiently dense and can be viewed as a continuum. A predictive dynamic user-optimal (PDUO) model has been previously used to model traffic flow with a given traffic demand distribution, in which travelers choose the routes that minimize the actual travel cost to the CBD. In this work, we combine the departure time choice with the PDUO model to study the simultaneous departure time and route choice problem. The user-optimal departure time principle is satisfied, which states that for each origin-destination (OD) pair, the total costs incurred by travelers departing at any time are equal and minimized. We then present an equivalent VI and solve it using the projection method after discretization based on unstructured meshes. A numerical experiment for an urban city with two CBDs is presented to demonstrate the effectiveness of the numerical algorithm.

Key words: predictive dynamic user-optimal model; simultaneous departure time and route choice; variational inequality; projection method; unstructured meshes

#### 1. Introduction

The traffic equilibrium problem recently developed in the literature can be divided into two approaches: discrete and continuum modeling. The discrete modeling approach, in which the road

network is made up of discrete road links, is a conventional method of analyzing a transportation system in detail (Sheffi 1984, Ma et al. 2015a,b). The continuum modeling approach focuses on the macroscopic characteristics of the traffic flow in networks. It assumes that the road network is dense and can thus be viewed as a continuum in which travelers can choose their routes in two-dimensional space. The characteristic variables, such as demand, cost, and flow intensity, can be represented by smooth mathematical functions (Vaughan 1987, Yang, Yagar and Iida 1994, Iida, Asakura and Yang 1991, Wong and Wong 2015, 2016). Compared with the discrete modeling approach, the continuum modeling approach has advantages in macroscopic studies with very dense transportation systems. First, it reduces the problem size for dense networks, which saves computational time and memory because the problem size depends on the method used to approximate the modeling region rather than on the actual network itself. Second, during the initial phase of planning and study, there is usually insufficient data for setting up a dense network for detailed analysis using the discrete modeling approach. Fewer data are required in the continuum model because it can be characterized by a small number of variables and does not require data for all links. Finally, the continuum modeling approach gives a better understanding of the global characteristics of a road network because the numerical results can be visualized in a two-dimensional sense. The continuum modeling approach is by no means a substitute for the discrete modeling approach, but it can be complementary, especially for the macroscopic modeling of a very dense transportation system (Ho and Wong 2006, Ho, Wong and Loo 2006).

The traffic equilibrium problem was initially studied from the static view, but this cannot take into account temporal variations and dynamic characteristics such as the travelers' departure time choices, dynamic route choices, and the evolution of traffic congestion. The dynamic traffic assignment (DTA) was therefore developed. The DTA problem includes two fundamental components: traffic flow and travel choice (Szeto and Lo 2006). Depending on the available route and departure time choices, DTA models can be divided into three types (Szeto and Wong 2012): pure departure time choice models (Small 1982), pure route choice models (Lo and Szeto 2002a,b, Lo and Chen 2000a,b, Tong and Wong 2000, Szeto, Jiang and Sumalee 2011), and simultaneous departure time and route choice models (Yang and Meng 1998, Friesz et al. 1993, Wie, Tobin and Friesz 1995, Szeto and Lo 2004, Ran, Hall and Boyce 1996, Han, Friesz and Yao 2013, Long et al. 2016, 2015, Ma, Ban and Pang 2016). However, most DTA models are confined to the discrete modeling approach, and can be formulated as nonlinear complementarity problems (Szeto and Lo 2004, Ban et al. 2012a,b), mathematical programming problems (Lo and Chen 2000a,b, Lo and Szeto 2002a, Yang and Meng 1998), fixed-point problems (Szeto, Jiang and Sumalee 2011), and variational inequality (VI) problems (Friesz et al. 1993, Wie, Tobin and Friesz 1995, Lo and Szeto 2002b, Szeto and Lo 2004, Ran, Hall and Boyce 1996, Huang and Lam 2002).

A simultaneous departure time and route choice model considers both of these aspects and is essentially a generalization of the pure route and pure departure time choice models. However, the continuum modeling approach has hitherto only been used to study the pure route choice problem. Tao et al. (2014) presented a city model in which the total cost of the whole traffic system was minimized. Jiang et al. (2014) developed a model for a polycentric city in which the instantaneous travel cost based on instantaneous information was minimized. Du et al. (2013) presented a predictive dynamic user-optimal (PDUO) model for a single CBD in which the predictive actual cost, based on the assumption that travelers had perfect future information about the traffic conditions, was minimized. Lin et al. (2015) extended the PDUO model to a polycentric city and constituted a numerical algorithm based on unstructured meshes. As an important component of travel behavior in DTA, the departure time choices of travelers are important to the dynamic evolution process of transportation. Given the total traffic demand at every location, the travelers choose their departure times following some equilibrium principle. Moreover, departure time choice must be considered in future extension work (e.g., integration of land use, transport and transport-related pollutants). However, departure time choice was not considered in any of the aforementioned dynamic continuum models.

VI formulations have received a great deal of attention in modeling a simultaneous departure time and route choice problem in the discrete modeling approach. Friesz et al. (1993) presented a continuous-time path-based VI model, and Han, Friesz and Yao (2013) discussed the existence of a solution to the VI by using a generalized Vickry model to simulate the network loading problem. Wie, Tobin and Friesz (1995) presented a discrete-time version of the VI formulation and a heuristic algorithm to solve it. Ran, Hall and Boyce (1996) presented a link-based VI model for the traffic equilibrium problem, but provided no algorithm to solve it. Huang and Lam (2002) proposed a heuristic algorithm to solve the presented VI model with queues. More recently, many studies have been carried out under the framework of differential variational inequality (DVI) (Pang and Stewart 2008). Based on the VI formulation in Friesz et al. (1993), Friesz and Mookherjee (2006) described the problem using the DVI, treated it as an equivalent fixed-point problem, and solved it using a projection algorithm. In Friesz et al. (2011), the DVI was further used to study both within-day and day-to-day dynamic equilibrium. Friesz et al. (2013) presented a DVI model in which the LWR model was adopted in the network loading procedure.

In this work, we combine the departure time choice with the PDUO model to study the simultaneous departure time and choice problem. In modeling, we define the user-optimal departure time condition mathematically, which states that, for each OD pair, the total cost incurred by travelers departing at any time are equal and minimized. Then, we prove the condition is equivalent to a continuous VI formulation, which has only been studied using the discrete modeling approach.

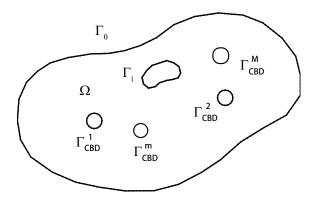


Figure 1 A polycentric urban city with an arbitrary configuration.

The existence of a solution to the VI problem is discussed. In the algorithm, the finite volume method and MSA are used to solve the PDUO model, which is the same as that in Lin et al. (2015). To solve the continuous VI, we first obtain the discrete VI problem after time and spatial discretization based on unstructured meshes. We then adopt the GLP projection method to solve the discrete VI formulation and use the gap function to measure the convergence. A numerical experiment for a polycentric city with two CBDs is given to demonstrate the effectiveness of the algorithm.

The remainder of this paper proceeds as follows. The description and context of the problem are given in Section 2. The PDUO model is introduced in Section 3. Section 4 presents the solution algorithm based on unstructured meshes. A numerical experiment for a polycentric city with two CBDs is presented in Section 5. The conclusions are given in Section 6.

## 2. Problem description

We consider a polycentric urban city with  $M(M \ge 2)$  compact CBDs (see Figure 1). The city region is  $\Omega$  and the boundary is  $\Gamma = \Gamma_0 \cup \Gamma_i \cup \Gamma_{CBD}^1 \cup \Gamma_{CBD}^m \cup \ldots \cup \Gamma_{CBD}^M$ , where  $\Gamma_0$  is the outer boundary,  $\Gamma_i$  is the boundary of an obstruction, and  $\Gamma_{CBD}^m$   $(m = 1, \ldots, M)$  is the boundary of the mth CBD. The travelers are classified into M classes according to the different CBDs. The city region is viewed as a continuum, and the travelers are generated and choose routes to their CBDs in the two-dimensional space. The modeling period  $T = [0, t_{end}]$ , where  $t_{end}$  is the time sufficient for all travelers to arrive the CBDs.

We denote the variables as follows.

•  $\rho^m(x,y,t)$   $(m=1,\ldots,M,$  in  $veh/km^2)$  is the density of the mth class of traffic flow at location (x,y) at time t.

•  $\mathbf{v}^m = (u^m(x,y,t), v^m(x,y,t)) \ (m=1,\ldots,M)$  is the velocity vector of the *m*th class of traffic flow at location (x,y) at time t.  $U^m(x,y,t) = |\mathbf{v}^m|$  (in km/h) is the speed of the *m*th class of traffic flow. This is determined by the sum of the densities at location (x,y) at time t, i.e.,

$$U^{m}(x,y,t) = U_{f}^{m}(x,y)e^{-\beta\rho^{2}(x,y,t)}, \ m = 1,\dots,M,$$
(1)

where  $U_f^m(x,y)$  (in km/hr) is the free-flow speed of the mth class of traffic flow at location (x,y),  $\rho(x,y,t) = \sum_{m=1}^{M} \rho^m(x,y,t)$ , and  $\beta$  is a positive parameter reflecting the road condition.

•  $\mathbf{F}^m = (f_1^m(x, y, t), f_2^m(x, y, t)) \ (m = 1, ..., M)$  is the flow vector of the mth class of traffic flow. The intensity of flow  $|\mathbf{F}^m|$  (in veh/km/hr) is defined as

$$|\mathbf{F}^{m}(x,y,t)| = \rho^{m}(x,y,t)U^{m}(x,y,t), \ m = 1,\dots,M.$$

- $\phi^m(x,y,t)$   $(m=1,\ldots,M,$  in \$) is the travel cost of the *m*th class of traffic flow from location (x,y) to the *m*th CBD.
- $T^m(x,y,t)$   $(m=1,\ldots,M,$  in hr) is the travel time of the mth class of traffic flow from location (x,y) to the mth CBD.
- $p^m(x,y,t)$   $(m=1,\ldots,M,$  in \$) is the schedule delay cost of the mth class of traffic flow departing from location (x,y) to the mth CBD at time t, which is a kind of penalty for late or early arrival. It is determined by the arrival time t+T(x,y,t).
- $C^m(x,y,t)$   $(m=1,\ldots,M,$  in \$) is the total cost of the mth class of traffic flow from location (x,y) to the mth CBD:

$$C^{m}(x,y,t) = p^{m}(x,y,t) + \phi^{m}(x,y,t).$$
(2)

•  $q^m(x,y,t)$   $(m=1,\ldots,M,$  in  $veh/km^2/hr)$  is the traffic demand of the mth class of traffic flow. The traffic demand satisfies the following conditions:

$$q^{m}(x,y,t) \geq 0, \forall (x,y) \in \Omega, \ t \in [0,t_{end}],$$
$$\int_{0}^{t_{end}} q^{m}(x,y,t) = q^{m}(x,y), \forall (x,y) \in \Omega,$$

where  $q^m(x,y)$  is the given total traffic demand of the mth class at location (x,y).

•  $c^m(x,y,t)$   $(m=1,\ldots,M,$  in \$/km) is the cost distribution of the mth class of traffic flow, which is defined as

$$c^{m}(x,y,t) = \kappa \left(\frac{1}{U^{m}(x,y,t)} + \pi^{m}(\tilde{\rho}(x,y,t))\right),\tag{3}$$

where  $\kappa$  (in \$/hr) denotes the value of time and  $\tilde{\rho}(x,y,t) = \{\rho^1(x,y,t), \dots, \rho^M(x,y,t)\}$ . The term  $\frac{\kappa}{U^m(x,y,t)}$  represents the travel time cost, and  $\kappa \pi^m(\tilde{\rho}(x,y,t))$  represents other related costs. For example, the high-density region is unattractive to travelers, and the perceived cost is related to the total density,  $\sum_{m=1}^{M} \rho^m(x,y,t)$ . Travelers also want to reduce conflicts with other classes of traffic flow (for the different travel directions and destinations) and the cost is related to the densities of all classes of traffic flow,  $\tilde{\rho}(x,y,t)$ .

Given the traffic demand distribution  $q^m(x, y, t)$ , we can model the traffic flow in the city and obtain the total cost  $C^m(x, y, t)$  through the PDUO model (Lin et al. 2015). Therefore, we denote  $C^m(x, y, t) = C^m(x, y, t, q)$ , where  $q = \{q^1(x, y, t), \dots, q^M(x, y, t)\}$ . We define for  $m = 1, \dots, M$ ,

$$C^{m}(x, y, q) = \min_{0 \le t \le t_{end}} C^{m}(x, y, t, q).$$

With these concepts, we give the following user-optimal departure time principle definition.

DEFINITION 1. The dynamic user-optimal departure time principle is satisfied if the following two conditions are satisfied for all  $(x, y) \in \Omega$  and m = 1, ..., M,

$$C^{m}(x, y, t, q) = C^{m}(x, y, q), \text{ if } q^{m}(x, y, t) > 0,$$
 (4)

$$C^{m}(x, y, t, q) \ge C^{m}(x, y, q), \quad \text{if } q^{m}(x, y, t) = 0,$$
 (5)

where  $q \in \bigvee$  and

$$\bigvee = \{q : q^m(x, y, t) \ge 0, \ m = 1, \dots, M, \ \forall (x, y) \in \Omega, \ \forall t \in [0, t_{end}];$$

$$\int_0^{t_{end}} q^m(x, y, t) dt = q^m(x, y), \ m = 1, \dots, M, \ \forall (x, y) \in \Omega \}.$$

The user-optimal conditions show that the total costs incurred by travelers departing at any time are equal and minimized, meaning a traveler cannot reduce his or her total cost by changing the departure time.

We then establish the equivalent variational inequality formulation of the user-optimal conditions.

Theorem 1. The user-optimal problem of Definition 1 is equivalent to the following variational inequality problem: find  $q^* \in \bigvee$  so that for all  $q \in \bigvee$ ,

$$\sum_{1 \le m \le M} \iint_{\Omega} \int_{0}^{t_{end}} C^{m}(x, y, t, q^{*}) (q^{m}(x, y, t) - q^{m*}(x, y, t)) dt d\Omega \ge 0.$$
 (6)

**Proof.** (Necessity.) If  $q^*$  satisfies the user-optimal conditions Eqs. (4)-(5). To prove that  $q^*$  is a solution for the VI problem, it is *sufficient* to show that for all  $(x, y) \in \Omega$ , m = 1, ..., M and  $q \in V$ ,

$$\int_0^{t_{end}} C^m(x, y, t, q^*) (q^m(x, y, t) - q^{m*}(x, y, t)) dt \ge 0.$$
 (7)

As  $\int_0^{t_{end}} q^m(x,y,t) - q^{m*}(x,y,t) dt = 0$ , it follows that Eq. (7) is equivalent to

$$\int_{0}^{t_{end}} (C^{m}(x, y, t, q^{*}) - C^{m}(x, y, q^{*}))(q^{m}(x, y, t) - q^{m*}(x, y, t))dt \ge 0.$$

Therefore, it is sufficient to show that for all  $(x,y) \in \Omega$ , m = 1, ..., M,  $t \in [0, t_{end}]$  and q,

$$(C^{m}(x, y, t, q^{*}) - C^{m}(x, y, q^{*}))(q^{m}(x, y, t) - q^{m*}(x, y, t)) \ge 0.$$
(8)

To do so, observe that if Eq. (8) fails for some  $t \in [0, t_{end}]$  and consider Eqs. (4) and (5), then  $q^m(x, y, t) - q^{m*}(x, y, t) < 0$ . Then we have

$$0 \le q^m(x, y, t) < q^{m*}(x, y, t) \Longrightarrow C^m(x, y, t, q^*) - C^m(x, y, q^*) = 0.$$

Hence Eq. (6) follows.

(Sufficiency.) Next, we suppose that  $q^* \in \bigvee$  satisfies Eq. (6) for all  $q \in \bigvee$ . Observe first from the definition of  $C^m(x, y, q^*)$ , the condition Eq. (5) is satisfied. It reminds us to prove Eq. (4). Assume that Eq. (4) is not satisfied at  $(x_0, y_0, t_0)$  for class  $m_0$ , then there exists a neighborhood of  $(x_0, y_0, t_0)$  so that

$$q^{m_0*}(x,y,t) > 0$$
,  $C^{m_0}(x,y,t,q^*) > C^{m_0}(x,y,q^*)$ .

Thus, there exists positive values  $\delta > 0$ ,  $\epsilon > 0$ ,  $\Omega_0$  and  $T_1$  so for  $(x, y) \in \Omega_0$  and  $t \in T_1$ ,

$$q^{m_0*}(x,y,t) > \delta$$
,  $C^{m_0}(x,y,t,q^*) > C^{m_0}(x,y,q^*) + 2\epsilon$ .

The continuity of  $C^{m_0}(x, y, t, q^*)$ , means that  $\epsilon_1 > 0$  exists, so for  $(x, y) \in \Omega_0$  and  $t \in T_2$ ,

$$C^{m_0}(x, y, t, q^*) < C^{m_0}(x, y, q^*) + \epsilon_1.$$

Here, without loss of generality, we assume that  $\epsilon = \epsilon_1$ ,  $|T_1| = |T_2|$ . Next, we construct a  $q \in \bigvee$  that contradicts Eq. (6). We define

$$q^{m}(x,y,t) = \begin{cases} q^{m*}(x,y,t) - \delta, & (x,y) \in \Omega_{0}, \ t \in T_{1}, \ m = m_{0}, \\ q^{m*}(x,y,t) + \delta, & (x,y) \in \Omega_{0}, \ t \in T_{2}, \ m = m_{0}, \\ q^{m*}(x,y,t), & otherwise. \end{cases}$$

If  $m = m_0, (x, y) \in \Omega_0, t \in T_1,$ 

$$q^{m*}(x,y,t) > \delta \Rightarrow q^m(x,y,t) = q^{m*}(x,y,t) - \delta \ge 0;$$

If  $m = m_0, (x, y) \in \Omega_0, t \in T_2$ ,

$$q^{m*}(x, y, t) \ge 0 \Rightarrow q^{m}(x, y, t) = q^{m*}(x, y, t) + \delta \ge 0;$$

Otherwise,

$$q^{m}(x, y, t) = q^{m*}(x, y, t) \ge 0.$$

We also have for  $m=m_0$ ,

$$\begin{split} & \int_{0}^{t_{end}} q^{m}(x,y,t)dt \\ &= \int_{[0,t_{end}]\backslash T_{1}\backslash T_{2}} q^{m}(x,y,t)dt + \int_{T_{1}} q^{m}(x,y,t)dt + \int_{T_{2}} q^{m*}(x,y,t)dt \\ &= \int_{[0,t_{end}]\backslash T_{1}\backslash T_{2}} q^{m*}(x,y,t)dt + \int_{T_{1}} q^{m*}(x,y,t) - \delta dt + \int_{T_{2}} q^{m*}(x,y,t) + \delta dt \\ &= \int_{0}^{t_{end}} q^{m*}(x,y,t)dt \\ &= q^{m}(x,y). \end{split}$$

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Thus  $q \in \bigvee$ . Then,

$$\sum_{1 \leq m \leq M} \iint_{\Omega} \int_{0}^{t_{end}} C^{m}(x, y, t, q^{*}) (q^{m}(x, y, t) - q^{m*}(x, y, t)) dt d\Omega$$

$$= \iint_{\Omega_{0}} \int_{T_{1} \cup T_{2}} C^{m_{0}}(x, y, t, q^{*}) (q^{m_{0}}(x, y, t) - q^{m_{0}*}(x, y, t)) dt d\Omega$$

$$= \iint_{\Omega_{0}} \left( -\delta \int_{T_{1}} C^{m_{0}}(x, y, t, q^{*}) dt + \delta \int_{T_{2}} C^{m_{0}}(x, y, t, q^{*}) dt \right) d\Omega$$

$$\leq \iint_{\Omega_{0}} \left( -\delta |T_{1}| (C^{m_{0}}(x, y, q^{*}) + 2\epsilon) + \delta |T_{2}| (C^{m_{0}}(x, y, q^{*}) + \epsilon) \right) d\Omega$$

$$= \iint_{\Omega} \left( -\delta |T_{1}| \epsilon \right) d\Omega$$

$$< 0.$$

This contradicts Eq. (6), and thus Eq. (4) is satisfied. Then, we may conclude that  $q^*$  satisfies the user-optimal conditions.

Gap functions have been used in many studies to evaluate the quality of the numerical solutions to traffic equilibrium problems (Long et al. 2015, 2016, Huang and Lam 2002, Lo and Chen 2000a). We define the gap function as

$$GAP = \sum_{1 \le m \le M} \iint_{\Omega} \int_{0}^{t_{end}} q^{m}(x, y, t) (C^{m}(x, y, t, q) - C^{m}(x, y, q)) dt d\Omega.$$

The gap function has the following properties:

- $GAP \ge 0$ , because  $q^m(x,y,t) \ge 0$  and  $C^m(x,y,t,q) \ge C^m(x,y,q)$  for all  $(x,y) \in \Omega$ , m = $1, \ldots, M, t \in [0, t_{end}].$
- $GAP = 0 \Leftrightarrow q$  is a solution of the VI problem (equivalently the user-optimal problem). If q is a solution of the VI problem, then for all  $(x,y) \in \Omega$ , m = 1, ..., M,  $t \in [0, t_{end}]$ , either  $q^m(x,y,t) = 0$  or

 $C^m(x,y,t,q)-C^m(x,y,q)=0$ , thus GAP=0. If GAP=0, then for all  $(x,y)\in\Omega$ ,  $m=1,\ldots,M$ ,  $t\in[0,t_{end}]$ , we have  $q^m(x,y,t)(C^m(x,y,t,q)-C^m(x,y,q))=0$ . Thus, if  $q^m(x,y,t)>0$ ,  $C^m(x,y,t,q)=C^m(x,y,q)$ . So GAP=0 is equivalent to that q and is a solution for the VI problem.

The gap function provides a measure of convergence in the VI problem (user-optimal problem). We use the relative gap function

$$RGAP = \frac{\sum\limits_{1 \leq m \leq M} \iint_{\Omega} \int_{0}^{t_{end}} q^m(x,y,t) (C^m(x,y,t,q) - C^m(x,y,q)) dt d\Omega}{\sum\limits_{1 \leq m \leq M} \iint_{\Omega} q^m(x,y) C^m(x,y,q) d\Omega}$$

as a stop condition of the numerical algorithm in Section 4.

In the discrete modeling approach, the existence of a solution to the continuous-time VI problem remains a fundamental and difficult issue. Zhu ahd Marcotte (2000) proved that when departure rates had uniform upper bounds, the VI problem had a solution. Han, Friesz and Yao (2013) established the existence of a solution to the VI problem by using the generalized Vickrey model for the dynamic network loading (DNL) without assuming a priori bounds on path flows. Proofs of the existence of a solution to the VI problem usually use the theorem given in Browder (1968). The difficult and key point of the proofs is to prove the continuity of the path delay operator and the compactness of the feasible region. In most of the discrete modeling approaches, the DNL is not described as nonlinear partial differential equations (PDEs) and this makes the analysis relatively easy. If nonlinear PDEs were used for the DNL (e.g., the LWR model), it would be difficult to investigate the existence of a solution. Friesz et al. (2013) used the LWR model for DNL and did not give the proof of the continuity of path delay operator except as a goal of future research. In this work, a two-dimensional LWR model is used, which is a more complicated way to study the existence of a solution. We believe the existence of a solution to the VI problem in the continuum modeling approach is meaningful and that it should be valuable to future work.

# 3. The predictive dynamic user-optimal model

In the user-optimal problem and the equivalent VI problem, the total cost  $C^m(x, y, t, q)$  should be given. In this section, we introduce the PDUO model, in which the travelers choose routes to minimize the travel cost under a given q, to compute the total cost  $C^m(x, y, t, q)$ .

We assume that travelers choose their routes to minimize the actual travel cost given the traffic demand distribution q. The predictive dynamic user-optimal principle is then satisfied, which states that the actual travel cost incurred by the used route is minimized. We introduce the following theorem about the route choice strategy (Du et al. 2013, Lin et al. 2015).

THEOREM 2. If  $(u^m, v^m)||(-\phi_x^m, -\phi_y^m)|$  (m = 1, ..., M), then the predictive dynamic user-optimal principle is satisfied.

#### 3.1. Model formulation

The predictive continuum dynamic user-optimal model includes the following two parts.

The conservation law part is

$$\begin{cases}
\rho_t^m + \nabla \cdot \mathbf{F}^m = q^m, & \forall (x, y) \in \Omega, \quad t \in T, \\
\mathbf{F}^m = -\rho^m U^m \frac{\nabla \phi^m}{|\nabla \phi^m|}, & \forall (x, y) \in \Omega, \quad t \in T, \\
\mathbf{F}^m(x, y, t) \cdot \mathbf{n} = 0, & \forall (x, y) \in \Gamma \setminus \Gamma_{CBD}^m, \quad t \in T, \\
\rho^m(x, y, 0) = \rho_0^m(x, y), & \forall (x, y) \in \Omega,
\end{cases}$$
(9)

Similar to mass conservation in fluid mechanics, for each class of traffic flow, the density, flow, and demand must satisfy the conservation law (the first equation of Eqs. (9)).  $\rho_0^m(x,y)$  is the initial density of the mth class of the traffic flow. The boundary condition  $\mathbf{F}^m(x,y,t) \cdot \mathbf{n} = 0$ ,  $\forall (x,y) \in \Gamma \setminus \Gamma_{CBD}^m$ ,  $t \in T$  means that no vehicle is allowed to enter the obstruction, the other CBDs, or leave the urban city. The velocity vector is chosen as  $\mathbf{v}^m = (u^m, v^m)||-(\phi_x^m, \phi_y^m) \ (m = 1, ..., M)$  to satisfy the predictive dynamic user-optimal principle.

#### The Hamilton-Jacobi part is

$$\begin{cases}
\frac{1}{U^m}\phi_t^m - |\nabla\phi^m| = -c^m, & \forall (x,y) \in \Omega, \quad t \in T, \\
\phi^m(x,y,t) = \phi_{CBD}^m, & \forall (x,y) \in \Gamma_{CBD}^m, \quad t \in T, \\
\phi^m(x,y,t_{end}) = \phi_0^m(x,y), & \forall (x,y) \in \Omega,
\end{cases}$$

$$(10)$$

where the initial condition of  $\phi_0^m(x,y)$   $(m=1,\ldots,M)$  is given by the Eikonal equation:

$$\begin{cases}
|\nabla \phi_0^m(x,y)| = c^m(x,y,t_{end}), & \forall (x,y) \in \Omega, \\
\phi_0^m(x,y) = \phi_{CBD}^m, & \forall (x,y) \in \Gamma_{CBD}^m.
\end{cases}$$
(11)

Here, we assume that there is no traffic at  $t = t_{end}$ , and that the travel cost is the instantaneous cost. The initial time is set at  $t = t_{end}$ , as the travel cost to a CBD only depends on the future situations. The Eikonal equation can be solved by using the fast marching method (see Jiang et al. (2009) for details).

#### 3.2. Travel time and the schedule delay cost

Next, we consider the travel time  $T^m(x,y,t)$  and the schedule delay cost  $p^m(x,y,t)$ . Along the used route (x(t),y(t)) satisfying  $\mathbf{v}^m = (u^m,v^m)||-(\phi_x^m,\phi_y^m)$ , we have

$$\frac{dT^m}{dt} = T_x^m \frac{dx(t)}{dt} + T_y^m \frac{dy(t)}{dt} + T_t^m = T_x^m u + T_y^m v + T_t^m.$$

According to the definition, we also have

$$\frac{dT^m}{dt} = -1.$$

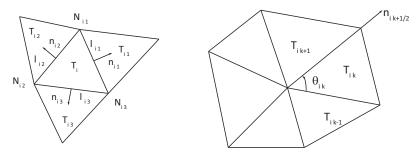


Figure 2 The unstructured meshes.

Thus,

$$T_t^m + T_x^m u + T_y^m v + 1 = 0.$$

Considering  $u^m = -U^m \frac{\phi_x}{\nabla \phi}$ ,  $v^m = -U^m \frac{\phi_y}{\nabla \phi}$ , we obtain the following equations to solve the travel time  $T^m(x, y, t)$ ,

$$\begin{cases}
T_{t}^{m} - \left(U^{m} \frac{\phi_{x}}{\nabla \phi} T_{x}^{m} + U^{m} \frac{\phi_{y}}{\nabla \phi} T_{y}^{m}\right) + 1 = 0, \\
T^{m}(x, y, t) = 0. \quad \forall (x, y) \in \Gamma_{CBD}, \quad t \in [0, t_{end}], \\
T^{m}(x, y, t_{end}) = T_{0}^{m}(x, y). \quad \forall (x, y) \in \Omega,
\end{cases}$$
(12)

where  $T_0^m(x,y)$  is solved by the following Eikonal equation

$$\begin{cases} |\nabla T_0^m(x,y)| = 1/U^m(x,y,t_{end}), & \forall (x,y) \in \Omega, \\ T_0^m(x,y) = 0, & \forall (x,y) \in \Gamma_{CBD}. \end{cases}$$

We assume that the mth class of travelers has a desired arrival time  $t^{m*}$  and some latitude to arrive early or late. We introduce the schedule delay function  $p^m(x, y, t)$ , which describes the penalty of early or late arrival. The function is defined as (Depalma et al. 1983):

$$p^{m}(x,y,t) = \begin{cases} \gamma_{1}((t^{m*} - \Delta) - (t + T^{m}(x,y,t))), & t + T^{m}(x,y,t) < (t^{m*} - \Delta), \\ 0, & (t^{m*} + \Delta) \le t + T^{m}(x,y,t) \le (t^{m*} + \Delta), \\ \gamma_{2}(t + T^{m}(x,y,t) - ((t^{m*} + \Delta))), & t + T^{m}(x,y,t) > (t^{m*} + \Delta). \end{cases}$$
(13)

Then, the total cost can be calculated by Eq. (2). In accordance with previous empirical results (Small 1982), we assume that  $\gamma_2 > \kappa > \gamma_1$ .

**Note.** In the PDUO model, travelers choose routes to minimize the travel cost (not the total cost). However, if the travel cost includes travel time only, the total cost is also minimized under the condition  $\gamma_2 > \kappa > \gamma_1$ . Here, the total cost is actually a monotonic function of the travel cost, and the predictive dynamic user-optimal principle states that the total cost incurred by the used route is minimized.

# 4. Solution algorithm

Here, we present the solution algorithm of the model formulated as the VI problem based on the unstructured meshes. We divide the city region  $\Omega$  with triangular meshes to handle the complex configuration. Let  $X_i$   $(i = 1, ..., N_P)$ ,  $T_i$   $(i = 1, ..., N_T)$  be a node and a triangle, respectively, within the domain, where  $N_T$ ,  $N_P$  are the number of triangles and nodes, respectively.  $A_i$ ,  $N_{ik}$ , and  $l_{ik}$  are the area, the kth node, and kth side of  $T_i$ , respectively.  $n_{ik}$  is the unit outer vector through the side  $l_{ik}$ . The kth neighboring triangle of  $T_i$  is denoted by  $T_{ik}$  (see Figure 2). We divide the time period  $[0, t_{end}]$  into N time steps and  $\Delta t = t_{end}/N$ .

## 4.1. Discrete variational inequality and the projection method

Based on spatial and time discretization, we write the VI problem into the following discrete VI problem. We denote  $(q^m)_i^n$ ,  $i = 1, ..., N_p$ , n = 1, ..., N is the traffic demand of the mth class in the node i and time step n and  $(q^m)_i$  is the total traffic demand of the mth class at node i. Then, the following constraint should be satisfied

$$\sum_{1 \le n \le N} (q^m)_i^n = (q^m)_i, \ m = 1, \dots, M, \ 1 \le i \le N_P.$$

$$(q^m)_i^n \ge 0, \ m = 1, \dots, M, \ 1 \le i \le N_P, \ 1 \le n \le N.$$

We define

$$\Lambda = \{ (q^m)_i^n : (q^m)_i^n \ge 0, \ m = 1, \dots, M, \ 1 \le i \le N_P, \ 1 \le n \le N; \sum_{1 \le n \le N} (q^m)_i^n = (q^m)_i, \ m = 1, \dots, M, \ 1 \le i \le N_P \}$$

We consider  $q^m(x, y, t)$  and  $C^m(x, y, t)$  as linear functions after the discretization based on the triangular meshes. We can then write the VI problem as the following discrete form.

(Discrete VI.) Find  $\mathbf{q}^* \in \Lambda$  so that for all  $\mathbf{q} \in \Lambda$ ,

$$\sum_{1 \le m \le M} \sum_{1 \le i \le N_P} \sum_{1 \le n \le N} (\tilde{C}^m)_i^n ((q^m)_i^n - (q^{m*})_i^n) \ge 0,$$

where  $(\tilde{C}^m)_i^n = \sum_{k=1}^{I_i} w_{ikj} (C^m)_{ikj}^n A_{ik} \Delta t$ ,  $I_i$  is the number of the elements around node  $X_i$ , ik is the index of the kth element of node  $X_i$ , ikj is the index of the jth node of element  $T_{ik}$ , and

$$w_{kj} = \begin{cases} \frac{1}{6}, & if \ ikj = i, \\ \frac{1}{12}, & otherwise. \end{cases}$$

We use the projection method to solve this. The following theorem holds.

THEOREM 3. Let  $\lambda > 0$ ,  $\mathbf{q}^*$  is a solution to the VI problem if and only if

$$\mathbf{q}^* = P_{\Lambda}(\mathbf{q}^* - \lambda \tilde{\mathbf{C}}(\mathbf{q}^*)),$$

where  $P_{\Lambda}(\mathbf{x})$  denote a unique projection of a vector  $\mathbf{x} \in \mathbb{R}^{M \times N_P \times N}$ , which is defined as

$$P_{\Lambda}(\mathbf{x}) = Argmin\{||\mathbf{y} - \mathbf{x}|| : y \in \Lambda\}.$$

Goldstein and Levitin and Polyak proposed the GLP projection algorithm as follows (Goldstein 1964, Levitin and Polyak 1966): given an initial  $\mathbf{q}_0$ , generate a sequence  $\{\mathbf{q}_k\}$  according to the following equation:

$$\mathbf{q}^{k+1} = P_{\Omega}[\mathbf{q}^k - \lambda_k \tilde{\mathbf{C}}(\mathbf{q}^k)], \tag{14}$$

where  $\lambda_k$  is a chosen positive step size, which should be set properly according to the specific problem.

Given the traffic demand distribution q, the total cost  $C^m(x,y,t,q)$  should be obtained by solving the PDUO model and travel time. The model includes two parts: the conservation equations and the Hamilton-Jacobi equations. Noting the different initial times of the two parts, we consider the solution procedure as a fixed-point problem. We use the finite volume method to solve both of these and the conventional MSA to solve the fixed-point problem (see Lin et al. (2015) for details). The formulations of travel time  $T^m(x,y,t)$  are also Hamilton-Jacobi equations, and we similarly solve them with the finite volume method. Then, the total travel cost is obtained by (2).

# 4.2. The complete solution algorithm

To solve the discrete VI problem using the GLP projection method, the projection  $P_{\Lambda}(\mathbf{p})$  should be given. By definition, solving the projection is equivalent to solve the following convex quadratic program:

$$\min z(\mathbf{q}) = ||\mathbf{q} - \mathbf{p}||$$

s.t.

$$\mathbf{q} \in \Lambda$$
.

We use the Frank-Wolfe method (Frank and Wolfe 1956) to solve the quadratic program. Given a feasible solution  $\mathbf{x}^k$ , then another feasible solution  $\mathbf{y}^k$ , we have approximately

$$z(\mathbf{y}^k) = z(\mathbf{x}^k) + \nabla z(\mathbf{y}^k)(\mathbf{y}^k - \mathbf{x}^k) = z(\mathbf{x}^k) + \nabla z(\mathbf{x}^k)\mathbf{y}^k - \nabla z(\mathbf{x}^k)\mathbf{x}^k.$$

To find the maximum drop from  $z(\mathbf{x}^k)$  to  $z(\mathbf{y}^k)$ , we solve the following linear optimization problem to find the descent direction  $\mathbf{y}^k - \mathbf{x}^k$ 

$$\min \nabla z(\mathbf{x}^k) \cdot \mathbf{y}^k \tag{15}$$

s.t.

$$\mathbf{y}^k \in \Lambda. \tag{16}$$

The solution procedure for solving the convex quadratic problem is summarized as follows.

# Algorithm A

- Step A1. Given an initial feasible solution  $\mathbf{x}^k$  and set k=1.
- Step A2. Find  $\mathbf{y}^k$  by solving the linear optimization problem (15) and (16) to get the descend direction  $\mathbf{y}^k \mathbf{x}^k$ .
  - Step A3. Find descent step size  $\lambda$  by solving  $\min_{0 \ge \lambda \ge 1} z(\mathbf{x}^k + \lambda(\mathbf{y}^k \mathbf{x}^k))$ .
  - Step A4. Set  $\mathbf{x}^{k+1} = \mathbf{x}^k + \lambda(\mathbf{y}^k \mathbf{x}^k)$ .
  - Step A5. If  $\frac{z(\mathbf{x}^k) z(\mathbf{x}^{k+1})}{z(\mathbf{x}^k)} \le \varepsilon$ , stop; otherwise go to Step A2.

In the case of discretization, the relative gap is

$$RGAP = \frac{\sum\limits_{1 \le m \le M} \sum\limits_{i} \sum\limits_{n} q_i^n (\tilde{C}_i^n - C_i)}{\sum\limits_{1 \le m \le M} \sum\limits_{i} q_i C_i} \times 100\%. \tag{17}$$

The complete solution algorithm for solving the discrete VI problem is as follows.

# Algorithm B

- Step B1. Given an initial arbitrary point  $\mathbf{q}^0 \in \Lambda$  and set k = 1.
- Step B2. Compute  $\mathbf{C}(\mathbf{q}^k)$ .
  - —Compute travel cost  $\phi^m$  by solving the PDUO model.
  - —Compute the travel time by solving the Eqs. (12).
- Compute the schedule delay  $p^m(x, y, t)$  through Eq. (13) and compute the total cost  $\tilde{\mathbf{C}}(\mathbf{q}^k)$  through Eq. (2).
  - Step B3. Compute  $\mathbf{q}^{k+1}$  through Eq. (14) by using Algorithm B.
- Step B4. Compute the relative gap RGAP through Eq. (17). If  $\frac{||\mathbf{q}^{k+1}-\mathbf{q}^k||}{||\mathbf{q}^k||} < \varepsilon_1$  and  $RGAP < \varepsilon_2$ , stop; otherwise set k = k+1 and go to Step B2.

# 5. Numerical experiments

We present a numerical example for an urban city with two CBDs to demonstrate the effectiveness of the numerical algorithm. The city (see Figure 3) spans about 37 km from west ( $x \approx 4 \ km$ ) to east ( $x \approx 41 \ km$ ) and 24 km from south ( $y \approx 10 \ km$ ) to north ( $y \approx 34 \ km$ ). CBD 1 and CBD 2 are located at (14 km, 20 km) and (31 km, 23 km), respectively, and the radiuses are 1 km. The destinations of Class 1 and Class 2 are CBD 1 and CBD 2, respectively. The modeling period is 6:00 a.m. to 11:00 a.m., i.e.,  $t \in [0 \ hr, \ t_{end}], \ t_{end} = 5 \ hr$ . We assume that travelers heading for the same CBD generally have similar desired arrival times regardless of their resident locations.

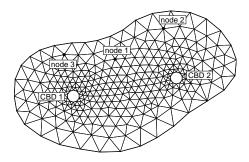


Figure 3 A polycentric urban city with two CBDs.

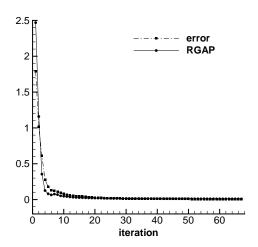


Figure 4 Convergence of the projection method.

We set  $\kappa = 72 \, \$/hr$ ,  $\gamma_1 = 48 \, \$/hr$ ,  $\gamma_2 = 108 \, \$/hr$ ,  $\Delta = 0.2 \, hr$  and the desired arrival times are  $t^{1*} = 2.8 \, hr$  and  $t^{2*} = 2.3 \, hr$ , respectively. The total travel demands of each class at location (x, y) are  $q^1(x, y) = 400 \, veh/km^2/hr$ ,  $q^2(x, y) = 450 \, veh/km^2/hr$ ,  $\forall (x, y) \in \Omega$ .

In Eq. (1), we set the parameter  $\beta = 2 \times 10^{-6}$ , and the free-flow speed is

$$U_f^m(x,y) = U_{max}^m \left( 1 + \gamma_2 \frac{d^1(x,y)}{d_{max}^1} \frac{d^2(x,y)}{d_{max}^2} \right),$$

where  $U^1_{max} = U^2_{max} = 65 \ km/hr$  is the maximum speed of Class 1 and Class 2,  $d^m(x,y)$  is the distance between (x,y) and the center of the mth CBD,  $d^1_{max} = \max_{(x,y) \in \Omega} d^1(x,y) \approx 27.6 \ km$ ,  $d^1_{max} = \max_{(x,y) \in \Omega} d^2(x,y) \approx 26.9 \ km$ , and  $\gamma_2 = 0.12 \ km^{-1}$ . In Eq. (3), we set

$$\begin{cases}
\pi^{1}(\tilde{\rho}(x,y,t)) = \pi_{0} \left( \frac{\rho^{2}(x,y,t)}{\rho^{1}(x,y,t) + \rho^{2}(x,y,t)} \right)^{2} + \pi_{1}(\rho^{1}(x,y,t) + \rho^{2}(x,y,t))^{2}, \\
\pi^{2}(\tilde{\rho}(x,y,t)) = \pi_{0} \left( \frac{\rho^{1}(x,y,t)}{\rho^{1}(x,y,t) + \rho^{2}(x,y,t)} \right)^{2} + \pi_{1}(\rho^{1}(x,y,t) + \rho^{2}(x,y,t))^{2},
\end{cases} (18)$$

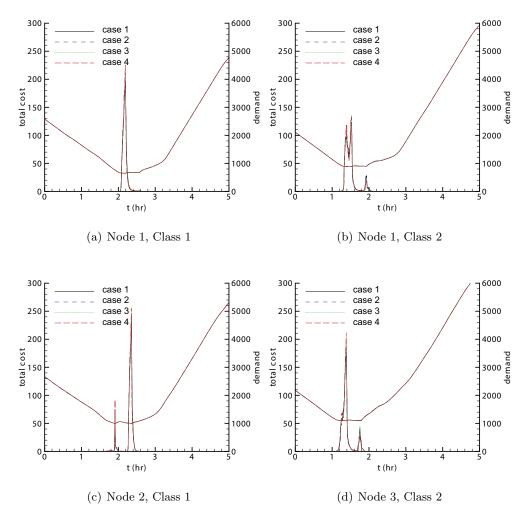


Figure 5 Demand and total cost in different cases.

where  $\pi_0 = 0.0025 \ hr/km$ ,  $\pi_1 = 10^{-8} \ h \ km^3/veh^2$ . The two terms in Eqs. (18) represent the preference for avoiding conflict with other classes of traffic flow and the preference for avoiding the high-density region, respectively.

We assume there is no traveler at the beginning of the modeling period and no cost incurred by entering each CBD. Thus, we have  $\rho_0^m(x,y) = 0$ ,  $\forall (x,y) \in \Omega$ , (m=1, 2) and  $\phi_{CBD}^m = 0$ , (m=1, 2). The modeling region is divided into triangular meshes with 298 nodes, 454 elements and 844 sides. To investigate the reasonableness of the algorithm numerically, we consider the cases with different numbers of time steps  $(N_t)$  and different initial traffic demand distributions  $(\mathbf{q}^0)$ . Specifically,

• Case 1:  $N_t = 1800$  and  $q^{1,0}(x,y,t) = q^1(x,y)g^1(t)$ ,  $q^{2,0}(x,y,t) = q^2(x,y)g^2(t)$ , where

$$g^{1}(t) = \begin{cases} t/4, & t \in [0 \ hr, \ 2 \ hr], \\ 1 - t/4, & t \in (2 \ hr, \ 4 \ hr], \\ 0, & t \in (4 \ hr, \ 5 \ hr], \end{cases} \qquad g^{2}(t) = \begin{cases} t/3, & t \in [0 \ hr, \ 1 \ hr], \\ 1/3, & t \in (1 \ hr, \ 3 \ hr], \\ (4 - t)/3, & t \in (3 \ hr, \ 4 \ hr], \\ 0, & t \in (4 \ hr, \ 5 \ hr]. \end{cases}$$

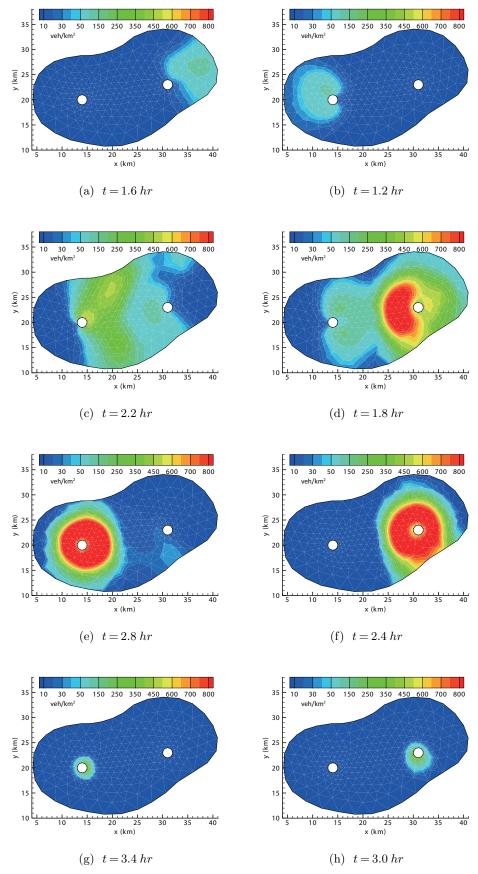


Figure 6 Density plot (left: Class 1; right: Class 2).

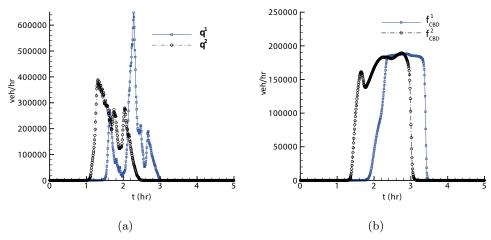


Figure 7 (a) Total demand; (b) Total inflow.

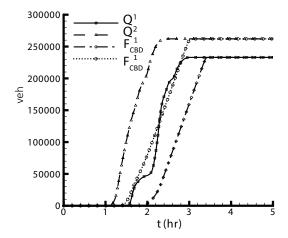


Figure 8 Cumulative demand and cumulative inflow.

- Case 2:  $N_t = 1800$  and  $q^{1,0}(x,y,t) = q^1(x,y)g^2(t)$ ,  $q^{2,0}(x,y,t) = q^2(x,y)g^1(t)$ .
- Case 3:  $N_t = 2700$  and  $q^{1,0}(x,y,t) = q^1(x,y)g^1(t)$ ,  $q^{2,0}(x,y,t) = q^2(x,y)g^2(t)$
- Case 4:  $N_t = 3600$  and  $q^{1,0}(x,y,t) = q^1(x,y)g^1(t)$ ,  $q^{2,0}(x,y,t) = q^2(x,y)g^2(t)$

In the GLP projection method, the step size is set  $\lambda_k = 30$  and the convergence threshold is  $\varepsilon_1 = \varepsilon_2 = 0.01$ . The convergence threshold in Algorithm B is  $\varepsilon = 10^{-9}$ . Figure 4 illustrates the error and RGAP of the GLP projection method (case 1), and we can see convergence after 67 iterations.

Figure 5 shows the demand and total cost at selected nodes (see Figure 3) in the city in the different cases. The numerical results with different numbers of time steps and different initial traffic demand distributions are almost the same, which shows the reasonableness of the solution algorithm. The user-optimal conditions are almost satisfied, and the total costs incurred by travelers departing anytime are almost equal and minimized. The distances between Node 1 and CBD 1

and between Node 1 and CBD 2 are nearly equal. However, the departure time of Class 1 is later than that of Class 2 because of the later desired arrival time [see Figures 5(a) and (b)]. Comparing Figures 5(a) and (c) [or Figures 5(b) and (d)], we find that for each class, the total cost is larger at the farther departure place. However, the departure time at the farther place is not always early [see Figures 5(a) and (c)] because the total cost of the early departure time may be greater due to traffic congestion. Case 2 is adopted for further discussion.

Figure 6 shows the density distribution of Class 1 and Class 2. We observe the traffic flow of Class 1. At t = 1.6 hr, for CBD 1 the travelers living far away start departing from home but have not yet arrived (see Figure 6(a)). At t = 2.2 hr, the travelers arrive at CBD 1 and traffic congestion has not yet been completely generated (see Figure 6(c)). At t = 2.8 hr, as the traveler numbers increase, the traffic flow is in a congestion condition around CBD 1 (see Figure 6(e)). At t = 3.4 hr, the traffic flow enters a free-flow state and almost all travelers have arrived at CBD 1 (see Figure 6(g)). The traffic flow of Class 2 has a similar evolution to Class 1 (see Figure 6(b), (d), (f), (h)).

The total demand of Class m over the whole domain at time t is

$$q^{m}(t) = \int \int_{\Omega} q^{m}(\phi^{m}(x, y, t), t) dx dy,$$

and the cumulative demand is

$$Q^{m}(t) = \int_{0}^{t} q^{m}(\xi)d\xi.$$

The total inflow of Class m through  $\Gamma^m_{CBD}$  is

$$f_{CBD}^m = \oint_{\Gamma_{CBD}^m} (\mathbf{F}^m \cdot \mathbf{n})(x, y, t) ds.$$

and the cumulative inflow is

$$F_{CBD}^{m} = \int_{0}^{t} f_{CBD}^{m}(\xi) d\xi.$$

The total demands, inflows, corresponding cumulative demands and corresponding cumulative inflows are shown in Figures 7 and 8. The departure and arrival times of Class 1 are in general later than those of Class 2, as the desired arrival time of Class 1 is later (Figure 7). For each class, the corresponding cumulative inflow is always lower than the corresponding cumulative demand, which describes a traffic delay. The two curves of each class finally coincide, which implies that all travelers have reached the CBDs (Figure 8).

# 6. Conclusions

A predictive continuum dynamic user-optimal model for the simultaneous departure time and route choice problem in a polycentric city is presented. Only pure route choice models have previously been developed, using the continuum modeling approach, and the departure time choice was not considered. Lin et al. (2015) extended the PDUO model to a polycentric city, in which the travelers choose their routes to minimize the actual travel cost. The current study combines the departure time choice with the PDUO model to examine the simultaneous departure time and route choice problem. This model satisfies the user-optimal departure time principle, which states that for each OD pair the total costs incurred by travelers departing at any time are equal and minimized. We establish the equivalent VI formulation of the problem and use the projection method to solve it, based on unstructured meshes. The PDUO model is solved by using the finite volume method and the MSA. The numerical results show that the user-optimal principle is satisfied, and the numerical algorithm is effective.

In this study, in modeling, we use the PDUO model to describe the evolution of traffic flow. This model is more complicated than the reactive dynamic user-optimal (RDUO) model, which is based on instantaneous traffic conditions. The PDUO model consists of two parts that are interconnected and the initial times are different. It is inherently challenging to solve it simply. In the algorithm, we use the most conventional projection method, GLP, to solve the VI problem. Other alternative projection methods can be developed to improve the efficiency in future work.

The existence of a solution to the VI problem using the continuum modeling approach is meaningful and should be valuable to future work.

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