



# Coupling control and human factors in mathematical models of complex systems

Roderick V.N. Melnik \*

M<sup>2</sup>NeT Laboratory, Wilfrid Laurier University, Waterloo Campus, 75 University Avenue West, Waterloo, ON, Canada N2L 3C5

## ARTICLE INFO

### Article history:

Received 27 May 2005

Received in revised form

19 February 2007

Accepted 31 October 2008

Available online 8 January 2009

### Keywords:

Complex dynamic systems

Coupled field theory

Systems science and cybernetics

Markov chains and decision analysis

Coupled multiscale phenomena

Human factors

Intelligent transportation systems and sustainability

Sequential analysis and Hamiltonian estimations

Changing environment and uncertainty

Perturbed generalized dynamic systems

## ABSTRACT

It is known that with the increasing complexity of technological systems that operate in dynamically changing environments and require human supervision or a human operator, the relative share of human errors is increasing across all modern applications. This indicates that in the analysis and control of such systems, human factors should not be eliminated by conventional formal mathematical methodologies. Instead, they must be incorporated into the modelling framework.

In this paper we analyse mathematically how such factors can be effectively incorporated into the analysis and control of complex systems. As an example, we focus our discussion around one of the key problems in the intelligent transportation systems (ITS) theory and practice, the problem of speed control, considered here as a decision making with limited information available. The problem is cast mathematically in the general framework of control problems and is treated in the context of dynamically changing environments where control is coupled to human factors. Since in this case control might not be limited to a small number of control settings, as it is often assumed in the control literature, serious difficulties arise in the solution of this problem. We demonstrate that the problem can be reduced to a set of Hamilton–Jacobi–Bellman equations where human factors are incorporated via estimations of the system Hamiltonian. In the ITS context, these estimations can be obtained with the use of on-board equipment like sensors/receivers/actuators, in-vehicle communication devices, etc. The proposed methodology provides a way to integrate human factors into the solving process of the models for other complex dynamic systems.

© 2008 Elsevier Ltd. All rights reserved.

## 1. Introduction

It is generally accepted that much of human intelligence can be characterized as the ability to recognize complex patterns, to analyse them and, if possible, to control. In this process the visual system, among others, together with cognition play a central role (Carroll, 2003, p. 11). In creating advanced technological systems human factors modelling must be incorporated as the processes of complex pattern recognition, their analysis, and ultimately control are intrinsically hierarchical. Many such systems are complex in a sense that they exhibit new properties, not easily deducible or found from properties of their individual parts. A number of examples of such systems and their mathematical treatments are discussed further in Section 5 based on the concept of coupling. Due to interactions of different parts in complex systems between themselves and with dynamically changing environment, coupled effects and phenomena are becoming increasingly important in studying such systems. Furthermore, giving the importance of

human factors in dealing with some such systems, in this contribution we demonstrate how human factors can be incorporated in mathematical models of complex systems on an important example from the intelligent transportation systems (ITS) theory—the problem of speed control. The main reason for this choice lies with the fact that while being strongly dependent on human factors, efficient speed control is known to be one of the key problems in the ITS technology (Endo et al. 1999a,b, 2000; Seto and Inoue, 1999). For the purpose of this paper we limit ourselves to three main technological analogies of human intelligence mentioned already, pattern recognition, analysis, and control. In the context of ITS technology such analogies are pertinent to (a) the application of information-driven functions (software for both control and computation) and (b) communications systems to controlling traffic (i.e. operating transport effectively, handling emergencies and incidents if they arise, automating driving and safety, etc.). These aspects are in the heart of the development of intelligent vehicles and highway systems (e.g., Gollu and Varaiya, 1998 and references therein).

Having specified our focus area from where all our examples will be drawn in the first four sections of this paper, we note further that our discussion will be pertinent to mathematical

\* Tel.: +1 519 884 1970x3662; fax: +1 519 884 9738.

E-mail address: [rmelnik@wlu.ca](mailto:rmelnik@wlu.ca)

models for the development of automated driving strategies based on a regulated speed control. Such strategies are important in many areas including collision avoidance (e.g., control the vehicle with respect to a vehicle running ahead, control the merging process into a main traffic stream where the “target” vehicle is running), the minimization of the fuel consumption, etc. Under the requirements of increased safety, minimization of the fuel consumption, and strict environmental constraints imposed by the government, many automotive and transport engineering companies have increased their attention to this problem (Endo et al. 1999a,b, 2000; Stotsky et al., 1995; Seto and Inoue, 1999; Butts et al., 1999; Fontaras and Samaras, 2007; Manzie et al., 2007). The increased complexity of ITS in this area and the successful development of automated driving strategies require accounting for human-related design factors and the integration of these factors into mathematical models used. These factors remain an important link in a chain of automated driving strategies developed from the application of mathematical models. Although there is no general model describing the dynamics of human interaction with complex systems in dynamically changing environment (Rouse et al., 1993; Goodrich and Boer, 2000), by analysing existing approaches applied previously to some model transport problems, in this paper we suggest a simple and efficient way to account for human factors in the solution of the speed control problem by considering a sequential Hamilton–Jacobi–Bellman (HJB)-equation-based approximation of the system Hamiltonian. Human-centred technologies are used frequently in many applications, including artificial intelligence (Shahar et al., 2006; Wren et al., 2006). As pointed out in Kessler and Knapen (2006), although much system development is still currently done by using a technology-centred approach (that is automating the functions the technology is able to perform), we witness an increasing-in-importance potential of human-centred design where we combine skilled human and automated support. This relatively new paradigm has already demonstrated its importance in complex system development where intervention of humans is still necessary on supervisory basis and/or at certain stages of system evolution (e.g., Mayer and Stahrea, 2006 and references therein). Nevertheless, the body of literature in this area is minimal (Barthelemy et al., 2002; Kraiss and Hamacher, 2001; Mayer and Stahrea, 2006), let alone mathematically rigorous developments.

From a methodological point of view the approach we develop in this contribution can be viewed as a blend of control and human factor aspects in the design/control of complex systems such as ITS, where we have to satisfy often competing requirements of human and technological objectives accounting for their capability limitations and constraints (Goodrich and Boer, 2000). The proposed approach is generic enough to be applicable to system developments in application areas outside of the ITS domain. Finally, we note that our approach has some common features paradigm of supervisory control (Kirlik et al., 1993; Melnik, 1997a) where, in the context of our problems, the control algorithm should respond in real time to changing conditions with the underlying process represented in a space of discrete events (Melnik, 1998a, 2008). Taking this point of view into account, we structure the rest of this paper as follows.

- In Section 2 we provide a general mathematical framework for controlling complex systems by using continuous and discrete control settings. The discussion is given in the context of the ITS speed control problem.
- In Section 3 we consider a specific example of the speed control problem subjected to the minimization of the fuel consumption.

- In Section 4 two important approaches to the development of automated driving strategies are discussed and difficulties in their computational implementation are analysed in detail with exemplification given for the problem considered in Section 3. In this section it is also shown that the general speed control problem can be reduced to a model based on the solution of HJB-type equations where human factors are incorporated naturally via estimations of the system Hamiltonian.
- In Section 5 we discuss complex systems and coupled problems in other areas of mathematical modelling and link this discussion with recently developed concept of perturbed generalized dynamic systems.
- Concluding remarks are given in Section 6.

## 2. Mathematical formulation of the control problem

While the formulation given in this section can be easily adapted to control of other complex systems, we exemplify our discussion here with an example concerning control of advanced vehicle systems. The model-based computer-aided control has become an intrinsic component of many technologies (Melnik and Melnik, 2000; Melnik and Roberts, 2001; Melnik and Jenkins, 2002; Melnik, 2003a; Huai et al., 2003; Xu et al., 2004; Wu et al., 2006, 2007; Wang and Melnik, 2007a, 2008c), and the ITS technology is not an exception. Due to the increased complexity and tight coupling of many different constraints imposed on the automotive systems development process, this control becomes increasingly important (Sivashankar and Sun, 1999). Such constraints come from the growing environmental and economic concerns leading to the rising customer expectations for fuel economy, performance, tightening emission, etc. There is a growing expectation that these constraints could be resolved by developing advanced transportation technologies (Kolmanovsky et al., 2000). Since many of these constraints are dependent strongly on the choice of driving strategies, this leads to the necessity of coupling control with human factors at the level of modelling rather than at the stage of system utilization. One of the concepts of interest in this context is human-centred automation, a relatively new concept that plays an increasingly important role in new technologies, both military and civil (Goodrich and Boer, 2000; Kraiss and Hamacher, 2001), where human factors are included into the synergetic integration of mathematical tools, embedded software engineering, and user-centred technologies (Angelov et al., 2003). While computers are in the heart of control of most complex man-designed systems, full automation is often either not feasible or not reasonable, in particular if system and/or environmental conditions are rapidly changing. In situations like this, function allocation and coupling between human factors and automation become critical (Kraiss and Hamacher, 2001). In this contribution, we demonstrate that this coupling can be treated formally via a sequential estimation of the system Hamiltonian, providing an important tool in theory and applications of ITS and other complex systems.

First, we formulate the problem of interest in the general framework of control problems providing all the explanations on an example of the analysis of the situation on the road during the interval time  $[0, T]$ , followed by the subsequent development of automated control strategies for road participants (driver-vehicle subsystems). This problem can be formulated as minimization of the following functional:

$$J(\mathbf{u}, \mathbf{v}) = \int_0^T f_0(\mathbf{x}(t), t, \mathbf{v}(t), \mathbf{u}(t)) dt \rightarrow \min, \quad (2.1)$$

where  $\mathbf{v}, \mathbf{u}$  are  $\mathbb{R}^m \rightarrow \mathbb{R}^m$  functions that represent the velocity and control of the entire dynamic system consisting of  $m$  subsystems

( $m \in \mathbb{N}$ , e.g. the number of vehicles), and the function  $f_0$  is the objective (problem-specific) function that could characterize fuel consumption, emissions, etc. (or a combinations of those quantities incorporated via corresponding weights). In (2.1)  $T$  is the prescribed (or estimated maximum) time, e.g. the time of reaching the final destination,  $\mathbf{v} = d\mathbf{x}/dt$ ,  $\mathbf{x}(t) = (x_1, x_2, \dots, x_m) \in \mathbb{R}^m$  is the position of the road participants at time  $t$  with applied (speed) control  $\mathbf{u}$ . The dynamics of coupling between the velocity and control is governed not only by (2.1) but also by the state constraints that are assumed to have the form of the equation of motion

$$\frac{d\mathbf{x}}{dt} = \mathbf{f}(\mathbf{x}, t, \mathbf{u}(t)) \quad (2.2)$$

and/or second Newton's law

$$\frac{d\mathbf{v}}{dt} = \mathbf{F}(\mathbf{x}, t, \mathbf{v}(t), \mathbf{u}(t)). \quad (2.3)$$

The vector functions  $\mathbf{f}$  and  $\mathbf{F}$  can be viewed as problem-specific approximations to the velocity function and acceleration (see e.g. Howlett, 1990; Stotsky et al., 1995 for some specific examples).

The qualitative (and quantitative) behaviour of the solution of this problem will be determined at a large extent by control constraints (Melnik, 1997a), defined here as

$$\mathbf{u}(\cdot) \in \mathcal{U}(t, \mathbf{x}), \quad (2.4)$$

where  $\mathcal{U}(t, \mathbf{x})$  is a given space–time set. It should be noted that for the solution of the speed control problem for transport engineering systems both groups of models, with continuous control and with discrete control, have been used in the literature (see, e.g., Howlett and Pudney, 1995 and references therein). Although models with continuous control have limited applicability in this context (moreover, their analysis typically requires the assumption of a finite number of control settings (Howlett, 1990)), they provide an important insight into more realistic models with discrete control. A major difficulty with the existing approaches based on continuous control models becomes apparent at the computational level where the quality of results depends heavily on the number and the form of *a priori* chosen control (traction) phases (e.g. power, coast, brake). A similar difficulty exists for models with discrete control settings, where the total number and locations of “switching control points” largely determines the quality of computational results. More precisely, the “switching control point” problem can be reduced to the determination of “optimal” times

$$0 = t_0 < t_1 < \dots < t_n \quad (2.5)$$

which correspond to such a partition of the vehicle trajectories  $\mathbf{x}^k = \mathbf{x}(t_k)$ ,  $k = 0, 1, \dots, n$  that control at those points makes the entire trip optimal in some specified sense. In conventional approaches, the responsibility on choosing the precise sequence of control settings and the determination of the “optimal” positions of these switching points can implicitly be shifted to the driver (Howlett, 1996). However, this becomes undesirable in the context of ITS where the driving strategy should be automated effectively to minimize the probability of accidents and to satisfy other goals of traffic control. Since the performance of the entire dynamic system can be improved greatly by increasing the number of discrete control settings, the ITS technology can provide an effective way to achieve these goals by implementing highly efficient driving control strategies on automated highway systems (AHS), a next generation of road systems that are intended to resolve various traffic issues (Seto and Inoue, 1999). Such driving strategies can be developed from the solution of problem (2.1)–(2.4) for a sufficiently high number  $n$  in (2.5). The practical implementation of such strategies for large  $n$  will require the

installation of on-board equipment such as actuators for controlling the breaks and throttle, LCX (leakage coaxial cable) receivers, as well as a laser radar and inter-vehicle communication devices. Then, in principle, the vehicles can be operated according to a vehicle velocity command (the indicated vehicle speed, road grade, road curvature, and accident information) received from the LCX cable installed alongside the road that allows for automatically maintaining a safe vehicle speed and headway distance. We emphasize that in this case, the definition of switching times (2.5) will be made sequentially on the basis of information accumulated by the given moment of time, as opposed to the conventional techniques based on one of the *a priori* choices of switching times.

An example involving one vehicle only is discussed in the next section in order to clarify the meaning of functions in general control problem (2.1)–(2.5) and to lay the foundation for further discussion of the key issues related to the solution of this problem in the context of ITS.

### 3. Conventional approaches on the example of vehicle speed control subjected to minimization of fuel consumption

The literature on different aspects of control of transportation systems is vast (e.g., Howlett and Pudney, 1995; Kolmanovsky et al., 2000; Qi and Zhao, 2005; Zhuan and Xia, 2006 to name just a few). A number of authors have attempted to apply different variants of continuity principle to determine switching control times (where, e.g., intervention of the driver is required). A continuity hypothesis found also its application in continuum (fluid-dynamics-like) approaches that have been developed for traffic flow models. In the latter case, such models rely frequently on unrealistic sets of assumptions and an *a priori* optimal velocity is one of them. More recently, several interesting contributions have been made to this area where authors realized that the underlying problem can be modelled with a hyperbolic system (with no conservation of momentum, e.g. Herty and Rascle, 2006 and references therein). However, the authors of these recent papers do not discuss control issues and that is where major challenges lie.

Let us explain the situation on an example of vehicle speed control subjected to the minimization of the fuel consumption. First note that in a number of practical situations the general formulation of problem (2.1)–(2.4) can be simplified considerably by assuming that control and state aspects of the dynamics of the moving vehicle could be decomposed (or factorized) in the objective function, i.e. if we assume that

$$f_0(\mathbf{x}, t, \mathbf{u}) = p[\mathbf{u}(t)] \cdot q[\mathbf{v}(t)], \quad (3.1)$$

where  $p$  and  $q$  are given functions. For example, according to Howlett (1990), for a problem where the total mechanical energy consumed by the vehicle is given by (2.1) and (3.1) and control is subject to the minimization of the fuel consumption, the above functions can be defined in the following forms (note that  $m$  is set to 1 in this case):

$$p \equiv u_+(t) = \frac{1}{2}[u(t) + |u(t)|], \quad q \equiv v(t). \quad (3.2)$$

As pointed out in Howlett (1990), Eq. (3.2) makes sense when a maximum applied acceleration is specified and that only positive acceleration consumes energy. We note further that specific forms of constraints (2.2) and/or (2.3) depend on the nature of the problem at hand, and since the vehicle dynamics can be influenced by the engine, automatic transmission, breaks and by many other factors, the constraints can appear to be fairly complex in the general case. Nevertheless, for a number of important situations state constraints can be reasonably

simplified. For example, it is often assumed that the control variable is the applied acceleration and that this variable can be determined as the difference between the “controlled” acceleration function  $s(u, v)$  (from a physical point of view this function can be interpreted as the driving controlled force per unit mass of the vehicle) and the “uncontrolled” deceleration function  $r(v)$  of the vehicle. In this case Eq. (2.3) takes the form

$$\frac{dv}{dt} = s[x, u(t), v(t)] - r[x, v(t)], \quad (3.3)$$

where possible dependency of functions  $s$  and  $r$  on the position  $x$  has also been included. This can be simplified further. Note that the form of the deceleration is again problem-specific depending on the need to account for a number of factors such as contributions of gravitational, aerodynamic, frictional and other forces. In the simplest case it can be approximated by the difference between the frictional resistance,  $r_0$ , and the gravitational component  $g$  in the direction of the vehicle motion (Howlett, 1996):

$$r[v(t)] = r_0[v(t)] - g(x). \quad (3.4)$$

Note also that (3.4) often takes the form of a quadratic law (so-called Davis' formula)

$$r[v(t)] = a + bv + cv^2, \quad a, b, c \in \mathbb{R}. \quad (3.5)$$

It is often the case that additional inequality constraints come naturally into the formulation of the problem. For example, the definition of the control variable might require further constraints such as positivity of the velocity and some control admissibility conditions (e.g. Howlett, 1990)

$$v(t) \geq 0, \quad |u(t)| \leq 1. \quad (3.6)$$

These constraints can be supplemented by additional constraints such as an upper limit on velocity. Inequality constraints (3.6) can be cast in the general vector form as

$$\mathbf{G} \leq \mathbf{0}, \quad \text{with } G_1 = -v, \quad G_2 = u^2 - 1. \quad (3.7)$$

Furthermore, some equality constraints might also be required. For example, if we assume that the trip has length  $L$ , this leads to the equality constraint expressed by the end-point reachability condition

$$\int_0^T v(t) dt = L, \quad (3.8)$$

supplemented by the boundary conditions

$$v(0) = v_1, \quad v(T) = v_2 \quad (3.9)$$

taken typically with  $v_1 = v_2 = 0$ .

Next, we note that the above example can be reformulated in the general framework (2.1)–(2.4) by introducing vector  $\mathbf{x} = (x_1, x_2)^T$  with  $x_1$  being the state variable, and  $x_2$  being the velocity of the vehicle. Indeed, since  $dx_1/dt = v$ , we can use (3.9) to derive that

$$x_1(T) - x_1(0) = L. \quad (3.10)$$

Then, taking into account (3.9) we have the initial and terminating conditions in the form

$$\mathbf{x}(0) = \mathbf{0}, \quad \mathbf{x}(T) = \mathbf{x}_T, \quad (3.11)$$

where  $\mathbf{x}_T = (L, 0)^T$ . We denote

$$\mathbf{f}(\mathbf{x}, t, \mathbf{u}(t)) = (x_2, s[x_1, x_2, u_2] - r[x_1, x_2])^T, \quad (3.12)$$

where  $u_2$  plays the role of  $u$  in the above example,  $\mathbf{u} = (0, u_2(t))^T$ , and take into account (3.7) and (3.11), i.e. only admit controls

$$\mathbf{u}(\cdot) \in \mathcal{U}(t, \mathbf{x}), \quad (3.13)$$

where

$$\mathcal{U}(t, \mathbf{x}) = \{\mathbf{u}(\cdot) \in \mathcal{U}^0(t) : \mathbf{x}_2(t) \geq 0, \quad \mathbf{x}(T) = \mathbf{x}_T, |u_2(t)| \leq 1\}. \quad (3.14)$$

Then, the definition of the objective function in the form (see (3.1))

$$f_0(\mathbf{x}(t), t, \mathbf{u}(t)) = [u_2(t)]_+ x_2(t) \quad (3.15)$$

completes the formulation of the vehicle speed control problem subjected to the minimization of the fuel consumption in the general framework (2.1)–(2.4).

Now, we are in a position to highlight major difficulties in applications of conventional methodologies to the above problem. First, we note that in reality the control variable of this problem cannot vary continuously due to the discrete character of the information (Melnik, 1998a) obtained in this specific case by the moving vehicle in a dynamically changing environment. Therefore, if we consider a finite (possibly very large) set of control settings, for example, throttle settings as it was originally proposed in Howlett (1990)

$$-1 = u^1 < u^2 < \dots < u^n = 1, \quad (3.16)$$

then the analysis of the problem can be reduced (under some severe assumptions such as “no speed limits”) to the consideration of four basic situations, as shown in Howlett (1990) (the acceleration, speedholding, coasting, and breaking phases), making use of quite specific forms of functions (3.2). In such cases it might be easier to define the objective function of the total fuel consumption accounting for these settings by splitting the total distance on an appropriate number of sub-intervals according to the discrete dynamic equation  $\mathbf{x}^k = \mathbf{x}(t_k)$  with

$$0 = \mathbf{x}^0 < \mathbf{x}^1 < \dots < \mathbf{x}^n = \mathbf{X} \quad (3.17)$$

and by assuming that the time  $\Delta t_{i+1} = t_{i+1} - t_i$  required to complete the segment trip  $[x_i, x_{i+1}]$  is known (or can be well approximated) for all  $i = 0, 1, \dots, n-1$  (see (2.5)). In most conventional approaches referenced here it is assumed that each control setting determines a constant rate supply. If we denote the fuel consumption and the control setting in the interval  $[x_i, x_{i+1}]$  by  $c_{i+1} \equiv c[u^{i+1}]$  and  $u^{i+1}$  ( $c = 0$  if  $u \leq 0$ ), respectively, the cost (fuel consumption) of the entire trip can be defined as (Pudney and Howlett, 1994; Howlett, 1996)

$$J = \sum_{i=0}^{n-1} c_{i+1} \Delta t_{i+1}. \quad (3.18)$$

First observe that since in the general case all control settings  $c_{i+1}$ ,  $i = 0, 1, \dots, n-1$  are functions of time, a more rigorous approach should be based on the consideration of functional (2.1) rather than function (3.18). We observe also that in some cases (including more realistic situations with speed limits), the development of automated (optimal or sub-optimal) driving strategies can be reduced to the analysis of simple combinations between a small number of control settings (e.g., power when  $u = 1$ , coast when  $u = 0$ , and break when  $u = -1$ ). However, due to the very nature of the control problem where we have to consider the ITS in a dynamically changing environment, a more detailed *sequential* analysis of the entire information sequence (3.16) is required. Such an analysis is intrinsic to other control problems where complex systems require human supervision or a human operator. The proposed methodology for this analysis is discussed in the next section.



#### 4. Sequential analysis of the global Hamiltonian keeps the key to efficient control of complex systems

In what follows, we shall demonstrate that a sequential analysis of the global Hamiltonian is essential in solving efficiently control problems involving complex systems.

In the context of our example, such a sequential analysis keeps the key to efficient driving strategies. First note that the information sequence for the decision making process obtained by on-board LCX receivers and by inter-vehicle communication devices always contains a certain degree of uncertainty. Indeed, some of the vehicle parameters, as well as the information on road conditions, can be known only partially (Stotsky et al., 1995). A complex dynamics of human performance in traffic systems (Rouse et al., 1993) brings along another factor that complicates the analysis of the entire dynamic system consisting of many driver-vehicle subsystems. This leads to a situation where control cannot be limited by a simple combination of basic settings, as we have discussed in the previous section, and a general approach should be developed to address the speed control problem in the ITS context.

The development of speed control strategies for ITS has become an important topic of research (Stotsky et al., 1995; Kiencke et al., 2006). In this section, our discussion focuses on a subset of the systems that consist of vehicles capable of measuring/estimating dynamic information from the target (typically, the immediate front) vehicle by its on-board sensors. The computers in the vehicles can process the measured data and generate proper throttling and breaking actions for controlling vehicles' movements under the constraints of safety, ride comfort, fuel minimization, etc. Recall that algorithms for speed control with constant acceleration/deceleration were developed and tested together with some simple algorithms for "approach" and "merging" control (Endo et al., 1999a). The authors of Endo et al. (1999a) developed linear models for passenger cars (in which any acceleration/deceleration can be generated according to the driver's operations Endo et al., 1999b) and generalized their results to a nonlinear model for heavy-duty vehicles where they accounted for transient responses (it is rather difficult to control the speed in this case, because of poor acceleration performance of such vehicles). As it was shown, it is necessary to account for saturation/delay in acceleration which could be an important characteristic of some vehicles. However, the results of simulations conducted in Endo et al. (1999a) showed that for long control periods, the model leads to unrealistic speeds, exceeding the target speed, and the maximum vehicle distance could become excessively long. In principle, such overshootings can be avoided by setting a short control period. However, since the dynamic behaviour of the vehicle model is intrinsically nonlinear and considerably complicated (Stotsky et al., 1995), in the general case it is necessary to take into account complex dependency between acceleration and speed of the vehicle using the general framework of (2.1)–(2.4).

In the reminder of this section we analyse three main approaches to the solution of the general speed control problem with exemplification given for the vehicle speed control subjected to the minimization of the fuel consumption, as considered in Section 3.

##### 4.1. The definition of the Hamiltonian via the solution of the adjoint problem

Some of the most powerful methodologies to the analysis of speed control problem are based on a heuristic application of the Pontryagin maximum principle. However, the application of these

methodologies to solving practical problems in the context of ITS requires overcoming a number of serious difficulties which will be considered below in the case where  $\mathbf{x} \in \mathbb{R}^2$  (see details after (3.9) in Section 3).

Applying formally the Pontryagin et al. (1986) maximum principle to the problem considered in Section 3 (problem (2.1)–(2.4) allows an analogous treatment), we can introduce a local Hamiltonian of the entire dynamic system in the following form:

$$H(\mathbf{x}(t), \mathbf{u}(t), \vec{\psi}(t), t) = -a_0 f_0(\mathbf{x}(t), \mathbf{u}(t), t) + \sum_{i=1}^2 \psi_i f_i, \quad (4.1)$$

where all notations come from the consideration of (2.1)–(2.4) in this special case,  $\mathbf{f} = (f_1, f_2)^T$ ,  $a_0$  is the normalization factor (Melnik, 1997a), while the adjoint vector-function  $\vec{\psi} = (\psi_1, \psi_2)^T$  is defined from the following adjoint system:

$$\frac{\partial \psi_i}{\partial t} = \frac{\partial f_0}{\partial x_i} - \sum_{k=1}^2 \psi_k \frac{\partial f_k}{\partial x_i} \quad \text{where } \psi_i(T) = 0, \quad i = 1, 2. \quad (4.2)$$

Then the result of the application of the Pontryagin et al. (1986) maximum principle to the speed control problem can be formulated as follows.

**Theorem 4.1.** *For a driving strategy determined by the pair  $(\mathbf{u}(t), \mathbf{x}(t))$  to be optimal it is necessary the existence of an adjoint vector-function  $\vec{\psi}(t)$  (components of which are not identical zero), defined by (4.2) such that*

$$\max_{\mathbf{u} \in \mathcal{U}} H(\vec{\psi}(t), \mathbf{x}(t), \mathbf{u}(t), t) = H(\vec{\psi}^*(t), \mathbf{x}^*(t), \mathbf{u}^*(t), t) \quad (4.3)$$

for almost all  $t \in [0, T]$ .

Practical difficulties with the application of this approach to the solution of the speed control problem for the ITS lie with the fact that state variables in this problem are not independent. This fact has led many authors to substantial simplifications of the problem (in particular, in the analysis of the system Hamiltonian) by considering a small subset of possible control settings (e.g., Howlett and Pudney, 1995). Unfortunately, this idea cannot be applied in the context of ITS, because both state variables are closely linked with the control function  $\mathbf{u}$ , and they might be decoupled in some special situations only.

Consider, as an example, the problem discussed in Section 3. In this case, functions participating in the definition of Hamiltonian (4.1) can be specified more precisely. Indeed, recall that in this case function  $f_0$  takes the form (3.15), while the vector function  $\mathbf{f}$  can be specified by its components as in (3.12). Clearly that even in this relatively simple case the state variables are coupled with the control by the following systems of equations:

$$\frac{\partial x_1}{\partial t} = x_2, \quad \frac{\partial x_2}{\partial t} = s[x_1(t), x_2(t), u_2(t)] - r[x_1(t), x_2(t)] \quad (4.4)$$

supplemented by the corresponding boundary conditions and other constraints previously discussed. In this case, according to (4.1) the Hamiltonian of the system can formally be written in the form

$$H = -a_0[u_2]_+ x_2 + \psi_1 x_2 + \psi_2 \{s[x_1, x_2, t, u_2] - r[x_1, x_2]\}. \quad (4.5)$$

For example, in a special case where  $s[x_1, x_2, t, u_2] = u_2$  and  $a_0 = 1$  (Howlett and Pudney, 1995), control can be confined to the following values  $u_2 = 1$ ,  $u_2 \in (0, 1)$ ,  $u_2 = 0$ ,  $u_2 \in (-1, 0)$  and  $u_2 = -1$  subject to the fulfilment of one of the following five relations: (a)  $\psi_2 > x_2$ , (b)  $\psi_2 = x_2$ , (c)  $0 < \psi_2 < x_2$ , (d)  $\psi_2 = 0$ , (e)  $\psi_2 < 0$ , respectively. Such a consideration takes the advantage of an implicit assumption on the possibility of decoupling state and control aspects of the problem. This leads to a substantial simplification of the analysis where we have to account for

control constraints (2.4). In the general case, the analysis cannot be reduced to five basic situations described above. Since the intersection between the set defined by control constraints and the set defined by state constraints is not empty (Melnik, 1997a), we note that even under these special assumptions, the key to the analysis of the Hamiltonian is kept by the coupled system of equations (4.2) and (4.4). Indeed, the adjoint function of the speed control problem considered in Section 3 is the solution of (4.2) which in the case where  $s$  equals  $u_2$  can be written in the following form:

$$\frac{d\psi_2(t)}{dt} - r'[v_0(t)]\psi_2 = \tilde{F}, \quad (4.6)$$

where

$$\tilde{F} \equiv \tilde{F}(v_0, u_0, f_0, \tilde{f}_2, \tilde{c}), \quad (4.7)$$

$\tilde{f}_2: \mathbb{R} \rightarrow \mathbb{R}$  is a real function associated with dynamically perturbed function  $F_2 = \partial f_2 / \partial x_2$ , and  $\tilde{a}_0 \in \mathbb{R}$  is a real constant that can be viewed as a dynamically perturbed parameter of normalization, subject to the dynamics of  $\psi_1$ . Getting a specific form of  $\tilde{F}$  requires a quite delicate analysis which was performed so far only for fairly simple cases (e.g. Howlett, 1990; Howlett and Pudney, 1995 and references therein). The determination of function  $\tilde{f}_2$  and constant  $\tilde{a}_0$  is also far from trivial and in the general case such a determination should be *adaptive*. Note also that  $(v_0, u_0)$  in (4.7) is assumed to be a fixed point associated with the optimal velocity of the vehicle and its optimal applied control which are not known *a priori*. However, if an approximate solution of problem (4.6) is found, then by using (4.1) a local (or pointwise) Hamiltonian function of the system can be defined. In this case, a major source of difficulties in constructive approximations of optimal driving strategies (that can be derived formally from minimizing the local Hamiltonian) lies with the intrinsically complex dynamics of the adjoint function and the adequate determination of the normalization factor. To proceed with such a construction the local Hamiltonian function should be integrated in time over the whole interval  $[0, T]$  which leads to the global Hamiltonian in the form

$$\mathcal{H}(u) = \tilde{H}_0 + \int_0^T H[x_1, x_2, t, u_2, \psi_1, \psi_2] dt, \quad (4.8)$$

where the actual value of  $\tilde{H}_0 \in \mathbb{R}$  depends not only on  $v_0$ ,  $L$ , and  $T$ , but also on the weight coefficients for implementing all remaining constraints of the problem. The optimal control strategies can now be determined by finding local minima of the Hamiltonian (4.8), but in practice this approach leads to serious computational difficulties due to too many degrees of freedom in (4.8). On the other hand, the problem can be reduced to the analysis of (4.1), e.g. by considering a small subset of basic control settings, only in quite simple cases such as those discussed in Howlett (1990).

#### 4.2. Using the embedding principle and the Lagrangian multipliers

In the context of ITS, more feasible computationally are approaches that are based on the embedding principle. First, we introduce the minimum cost function as follows:

$$J^*(\mathbf{x}(t), t) = \min_{\mathbf{u}(\tau) \in \mathcal{U}, t \leq \tau \leq T} \left\{ \int_t^T f_0(\mathbf{x}(\tau), \mathbf{u}(\tau), \tau) d\tau \right\}, \quad (4.9)$$

where  $0 \leq t \leq T$  and  $\mathbf{f}_0$  is defined in the context of the problem discussed in Section 3. Then, it appears that if the derivative of  $J^*$  with respect to  $\mathbf{x} = (x_1, x_2)$  exists, we can introduce a local Hamiltonian of the system as follows:

$$H = -a_0 f_0 + J_{x_1}^* x_2 + J_{x_2}^* f_2. \quad (4.10)$$

In this representation we accounted for state constraints (2.2) and (2.3) which in the context of problem discussed in Section 3 have the form (4.4). Accounting for control constraints (3.6) is straightforward (Howlett, 1996)

$$\mathcal{H} = H + \lambda(u_2 - 1) + \mu(-u_2 - 1), \quad (4.11)$$

where  $\lambda$  and  $\mu$  can be identified with the Lagrangian multipliers. For this specific case, the definition of the Hamiltonian in form (4.11) limits the number of degrees of freedom to two (see details of this approach in Pudney and Howlett, 1994) where the objective function was taken in form (3.18)). However, practical applications of this approach in the context of complex dynamic systems are limited due to the discrete nature of control in such problems which leads to non-existence of derivative  $\partial \mathcal{H} / \partial u$  in the classical sense. If, however, a formal operation of differentiation is performed, it is easy to conclude that

$$\frac{\partial \mathcal{H}}{\partial u_2} = \frac{\partial H}{\partial u_2} + \lambda - \mu, \quad (4.12)$$

where all the derivatives above and hereafter in the text should be understood in a generalized sense. Under some simplifying assumptions this formal approach can be applied to the speed control problem discussed in Section 3 for which the formal differentiation leads to the following result (Howlett and Pudney, 1995; Howlett, 1996):

$$\frac{\partial \mathcal{H}}{\partial u} = \begin{cases} x_2 + J_{x_2}^* + \lambda - \mu, & 0 < u_2 \leq 1, \\ J_{x_2}^* + \lambda - \mu, & -1 \leq u_2 < 0. \end{cases} \quad (4.13)$$

In this case, similar to our discussion in Section 4.1, further analysis can be reduced to the consideration of five different cases, depending on the mutual location of  $x_2$ , 0 and  $x_2 + J_{x_2}^*$  (Howlett, 1996). From a computational point of view this approach could be efficient in computing critical speeds for automated driving strategies, but in the general case it has the same limitations as the approach described in Section 4.1. Of course, in the case of simple control constraints (such as (3.6)), having the optimal velocity  $v_0(t)$ , it is a standard procedure to determine the optimal control (acceleration)  $u_0(t)$  by minimizing the (local) Hamiltonian function. Since the velocity is strongly coupled to control settings over the whole time interval (neither velocity nor control can be given *a priori*  $\forall [0, T]$ ), practical implementation of this procedure is problematic in the general case. Strictly speaking, in order to determine the optimal velocity and control globally, one needs to know the Hamiltonian which in its turns depends on those functions (Melnik, 1997a). However, formally the Hamiltonian (or Lagrangian due to the duality principle) can be defined locally provided the coupled system of equations (4.2) and (4.4) is solved. Alternatively, we have to solve the coupled system of equations in the Hamiltonian canonical form

$$\frac{d\mathbf{x}^*(t)}{dt} = \frac{\partial H}{\partial \vec{\psi}}(\mathbf{x}^*(t), \mathbf{u}^*(t), \vec{\psi}^*(t), t), \quad (4.14)$$

$$\frac{d\vec{\psi}^*(t)}{dt} = -\frac{\partial H}{\partial \mathbf{x}}(\mathbf{x}^*(t), \mathbf{u}^*(t), \vec{\psi}^*(t), t), \quad (4.15)$$

with the function  $H$  defined as

$$H(\mathbf{x}(t), \mathbf{u}(t), \vec{\psi}(t), t) \equiv f_0(\mathbf{x}(t), \mathbf{u}(t), t) + [\vec{\psi}(t)]^T \mathbf{f}(\mathbf{x}(t), \mathbf{u}(t), t). \quad (4.16)$$

Then, as follows from Theorem 4.1 for the optimality of control  $\mathbf{u}^*(t)$  and trajectory  $\mathbf{x}^*(t)$  the following inequality:

$$H(\mathbf{x}^*(t), \mathbf{u}^*(t), \vec{\psi}^*(t), t) \leq H(\mathbf{x}(t), \mathbf{u}(t), \vec{\psi}(t), t) \quad (4.17)$$

should hold for all  $\mathbf{u}(\cdot) \in \mathcal{U}$ , where  $\mathcal{U}$  is defined by (2.4). It is well-known that under sufficient smoothness assumptions (Kirk, 1970; Lions, 1982), the adjoint function and the optimal performance

measure are connected by

$$\vec{\psi}(t) = \frac{\partial J^*}{\partial \mathbf{x}}(t, \mathbf{x}^*(t)), \quad (4.18)$$

and hence the function  $H$  in (4.16) can be re-written in the form

$$H(\mathbf{x}(t), \mathbf{u}(t), \nabla J^*, t) \equiv f_0(\mathbf{x}(t), \mathbf{u}(t), t) + [\nabla J^*(\mathbf{x}(t), t)]^T \mathbf{f}(\mathbf{x}(t), \mathbf{u}(t), t). \quad (4.19)$$

In this case the dynamics of system perturbations (including those caused by human factors) is accommodated formally in the derivative of the performance measure. Since complex dynamic systems such as ITS exhibit an intrinsic interplay between state and control aspects of the dynamics, this accommodation does not preclude us from non-uniqueness of the solution of the resulting model. Indeed, following Pudney and Howlett (1994) let  $V_j$  be the speed of the vehicle at location  $x^j$ ,  $W_j$  be the limiting speed for control setting  $u^j$ , and  $U_j$  be the speed at location  $X_j$ , where it is assumed that the speed limits are changed at distances

$$0 = X_0 < X_1 < \dots < X_p = X. \quad (4.20)$$

Then, triple  $(U_j, V_j, W_j)$  can be obtained by using the Lagrangian multipliers under simplified assumptions of only three control settings,  $u = 1$ ,  $u = 0$ , and  $u = -1$ . This triple defines critical speeds for the interval  $(X_{j-1}, X_j)$  such that  $0 \leq U_j \leq V_j \leq W_j \leq M_j$  (Pudney and Howlett, 1994). However, the quality of the “speed-holding” phase approximation by using, for example, coast-power control pairs on each such interval depends strongly on the number of control pairs (denoted here by  $s_j$ ) for this interval. In fact, in the general case only in the limit  $s_j \rightarrow \infty$  we can obtain a unique holding speed for this interval and to avoid undesirable vehicle speed oscillations between control switchings (e.g. between values  $V_j < M_j$  and  $V_j = \min\{W_j, M_j\}$  subject to  $s_j$ , see the results of computational experiments in Pudney and Howlett, 1994).

Despite these difficulties, the problem of speed control in its general framework can be formalized by writing down the full system of Kuhn–Tacker necessary conditions and by including all constraints in the globally defined generalized Lagrangian function (or Hamiltonian, as follows from the duality principle). Let us consider this approach in some details. Provided  $\mathcal{H}$  possesses sufficient smoothness, the minimization of (4.11) is a standard problem in optimization theory, and the necessary conditions of control optimality will follow from  $\partial H / \partial u = 0$  (Kirk, 1970; Sucharev et al., 1989). This idea is easy to apply in those cases where control constraints are given *a priori* in a relatively simple form (Howlett and Pudney, 1995). However, addressing the speed control problem in the general case and accounting for a complex dynamic interplay between state and control constraints is a much more difficult task. For example, in the case discussed in Section 3 this problem is reducible to the following constrained optimization problem:

$$H(\mathbf{x}(t), \mathbf{u}(t), \nabla J^*, t) \rightarrow \min \quad (4.21)$$

$$g_i(t) \leq 0, \quad i = 1, 2, 3, \quad g_i(t) = 0, \quad i = 4, 5, \quad (4.22)$$

(see (3.15), (4.9), (4.19)), subject to the following constraints:

$$g_1(t) = u_2(t), \quad g_2(t) = -u_2(t) - 1, \quad g_3(t) = -x_2(t), \quad (4.23)$$

$$g_4(t) = x_1(T) - L, \quad g_5(t) = x_2(T). \quad (4.24)$$

Then, by using classical Lagrangian multipliers for the equality constraints together with relaxing variables  $\gamma_i^2$ ,  $i = 1, 2, 3$  for the inequality constraints, we can define the generalized Lagrangian function in the following form (Sucharev et al., 1989):

$$L(\mathbf{x}(t), \mathbf{u}(t), t, \vec{\lambda}, \vec{\gamma}) = H + \sum_{i=1}^3 \lambda_i [g_i(t) + \gamma_i^2] + \sum_{i=4}^5 \lambda_i g_i(t), \quad (4.25)$$

where vector  $\vec{\lambda}$  is the vector of Lagrangian multipliers. The Kuhn–Tacker necessary conditions for the extremum of this function are

$$\frac{\partial L}{\partial t} = 0, \quad \frac{\partial L}{\partial u_2} = 0, \quad \frac{\partial L}{\partial x_i} = 0, \quad i = 1, 2, \quad (4.26)$$

$$\frac{\partial L}{\partial \lambda_i} = 0 \iff g_i(t) \leq 0, \quad i = 1, 2, 3,$$

and

$$g_i(t) = 0, \quad i = 4, 5, \quad (4.27)$$

$$\frac{\partial L}{\partial \gamma_i} = 0 \iff \lambda_i g_i(t) = 0, \quad i = 1, 2, 3, \quad (4.28)$$

and, finally

$$\lambda_i \geq 0, \quad i = 1, \dots, 5. \quad (4.29)$$

In order to find the solution of the speed control problem we should solve coupled system (4.26)–(4.29) with respect to unknown variables,  $x_1, x_2, u_2, \lambda_i$ . Since control cannot be found globally based on a locally defined velocity function, this system should be solved in an adaptive manner. Note that system (4.26)–(4.29) can be simplified substantially in some special cases, for example when local (rather than global) solutions are sought and/or  $s$  in the state equation (3.3) is a linear function of control (Howlett, 1990; Howlett and Pudney, 1995). Such simplified considerations allow us to reduce the analysis of the Hamiltonian/Lagrangian to a small number of control settings, as it has been explained earlier in this section. Attempts to apply such methodologies to the general speed control problem are confronted with serious difficulties. These difficulties are convenient to explain at the computational level for the problem from Section 3.

Consider a trajectory of the vehicle with  $n$  distinct phases

$$P_i = (x^i, x^{i+1}), \quad i = 0, 1, \dots, n-1, \quad x^0 = 0, \quad x^n = X, \quad (4.30)$$

each with certain speed limits  $M_{j+1}$ , and the number  $s_{j+1}$  of control pairs inside of each speed limit interval  $(X_j, X_{j+1})$  (for example, “coast-power” pairs to approximate the speed-holding phase, etc. as argued, e.g., in Pudney and Howlett, 1994)

$$(M_{j+1}, s_{j+1}), \quad x \in (X_j, X_{j+1}), \quad j = 0, 1, \dots, p-1, \quad (4.31)$$

where  $X_0 = x^0$  and  $X_n = x^n$ .

Then, we ask the following question: What values of  $n$  and  $p$  should be chosen to approximate effectively the optimal trip? A simple way would be to choose these values to satisfy the distance and time constraints following the technique described in Howlett (1990) (e.g. p. 468), and then to determine Lagrangian multipliers by using methodology of (Pudney and Howlett, 1994). However, this way cannot guarantee global optimality, because additional constraints that appear in the amended formulation of the problem (such as speed limits and an *a priori* pre-defined number of control pairs) should be included in the definition of the Hamiltonian (Lagrangian), but they are not. If we include these constraints into the definition of the Hamiltonian/Lagrangian, the analysis cannot be reduced to only those five cases discussed previously in this section. In the general case, the number of speed holding phases for the entire trip can be determined by *a posteriori* estimations based on a sequential algorithm of information processing, accounting for human factors (Melnik, 1998a). Recall that in conventional methodologies this number is postulated *a priori*. At the same time, Lagrangian multipliers (see (4.11)–(4.13)) can determine only critical speeds within each interval (4.31). Algorithms for the solution of the general speed control problem

can be constructed if we take into account that the speed  $V_k$ ,  $k = 1, \dots, n-1$  at location  $x^k$  for arbitrary (large)  $n$  depends primarily on the behaviour of the system on  $\Delta x_1, \dots, \Delta x_k$ , where  $\Delta x_i = x^i - x^{i-1}$ . We formalize this idea of the Markovian-type controlled dynamics below by using Hamiltonian estimations. This allows us to couple control with human factors within a general mathematical framework. Note that the model of the system as well as the objective function for the minimization as well as constraints are subject to uncertainties as a result of dynamically changing conditions in which the system operates. Due to such uncertainties, the resulting control strategies may not be optimal in the entire time interval in a classical sense. However, they are optimal within each time interval where the same Hamiltonian estimation is used.

#### 4.3. Hamiltonian estimations and human factors

It is often the case that effective human-centred automation is a necessary element of a well-designed controlled ITS. Of course, it is not necessarily a sufficient element for an optimal performance of the overall system (Kirluk et al., 1993). However, if human factors are incorporated into a mathematical model, then efficient control of the overall system based on human-centred automation often becomes a key tool in improving system performance.

Recall that by (4.9) we introduced the minimum cost function. This function is based on a performance measure that allows us to include our speed control problem in a larger class of problems by considering the following functional:

$$J(\mathbf{x}(t), t, \mathbf{u}(\tau) : t \leq \tau \leq T, \mathbf{u} \in \mathcal{U}) = \int_t^T f_0(\mathbf{x}(\tau), \tau, \mathbf{u}(\tau)) d\tau, \quad (4.32)$$

where  $t$  can be any value from the closed interval  $[0, T]$  and  $\mathbf{x}(t)$  can be any admissible state value. Now we can follow a general path of the dynamic programming approach (Kirk, 1970; Sucharev et al., 1989). Since our aim is to determine the control that minimizes (4.32) for any admissible  $\mathbf{x}(t)$  and for any  $t \in [0, T]$ , we note that the minimum cost function for this problem can be re-written by subdividing the intervals

$$J^*(\mathbf{x}(t), t) = \min_{\mathbf{u}(\tau) \in \mathcal{U}, t \leq \tau \leq T} \left\{ \int_t^{t+\Delta t} f_0 d\tau + \int_{t+\Delta t}^T f_0 d\tau \right\}. \quad (4.33)$$

From the embedding principle used in the dynamic programming approach (e.g. Kirk, 1970; Sucharev et al., 1989) and relationships (4.9) and (4.33) we have

$$J^*(\mathbf{x}(t), t) = \min_{\mathbf{u}(\tau) \in \mathcal{U}, t \leq \tau \leq t+\Delta t} \left\{ \int_t^{t+\Delta t} f_0 d\tau + J^*(\mathbf{x}(t+\Delta t), t+\Delta t) \right\}, \quad (4.34)$$

where  $J^*(\mathbf{x}(t+\Delta t), t+\Delta t)$  is the minimum cost of the trip for the time interval  $t+\Delta t \leq \tau \leq T$  with the “initial” state  $\mathbf{x}(t+\Delta t)$ . Applying now formally Taylor’s series expansion in (4.34) about point  $(\mathbf{x}(t), t)$ , we have

$$\begin{aligned} J^*(\mathbf{x}(t), t) = & \min_{\mathbf{u}(\tau) \in \mathcal{U}, t \leq \tau \leq t+\Delta t} \left\{ \int_t^{t+\Delta t} f_0 d\tau \right. \\ & + J^*(\mathbf{x}(t), t) + \left( \frac{\partial J^*}{\partial t}(\mathbf{x}(t), t) \right) \Delta t + \left[ \frac{\partial J^*}{\partial \mathbf{x}}(\mathbf{x}(t), t) \right]^T \\ & \times [\mathbf{x}(t+\Delta t) - \mathbf{x}(t)] + o(\Delta t) \left. \right\}. \end{aligned} \quad (4.35)$$

Then, using the main property of the Landau symbol, taking into account Eq. (2.2) for  $\Delta t \rightarrow 0^+$ , and dividing (4.35) by  $\Delta t$ , we obtain

$$\begin{aligned} 0 = & \frac{\partial J^*}{\partial t}(\mathbf{x}(t), t) + \min_{\mathbf{u}(t) \in \mathcal{U}} \left\{ f_0(\mathbf{x}(t), \mathbf{u}(t), t) \right. \\ & + \left[ \frac{\partial J^*}{\partial \mathbf{x}}(\mathbf{x}(t), t) \right]^T [\mathbf{f}(\mathbf{x}(t), \mathbf{u}(t), t)] \left. \right\}. \end{aligned} \quad (4.36)$$

Further, it is easy to see that if we set  $t = T$  in (4.9) we get

$$J^*(\mathbf{x}(T), T) = 0. \quad (4.37)$$

If we now define the system Hamiltonian by (4.19) and take into account that the optimal minimizing control depends on  $\mathbf{x}$ ,  $\partial J^* / \partial \mathbf{x}$  and  $t$

$$\mathcal{H} \left[ \mathbf{x}(t), \mathbf{u}^* \left( \mathbf{x}(t), \frac{\partial J^*}{\partial \mathbf{x}}, t \right), \frac{\partial J^*}{\partial \mathbf{x}}, t \right] = \min_{\mathbf{u}(t) \in \mathcal{U}} \mathcal{H} \left( \mathbf{x}(t), \mathbf{u}(t), \frac{\partial J^*}{\partial \mathbf{x}}, t \right), \quad (4.38)$$

we arrive at a mathematical model for the speed control problem (2.1)–(2.4) represented in the form of the HJB equation

$$0 = \frac{\partial J^*}{\partial t}(\mathbf{x}(t), t) + \mathcal{H} \left[ \mathbf{x}(t), \mathbf{u}^* \left( \mathbf{x}(t), \frac{\partial J^*}{\partial \mathbf{x}}, t \right), \frac{\partial J^*}{\partial \mathbf{x}}, t \right] \quad (4.39)$$

and supplemented by condition (4.37). The solution to this problem is understood in the generalized sense (Lions, 1982; Melnik, 1997a). Naturally, it cannot be reduced to the five cases discussed before. Instead, a sequential (in real time) algorithm is required to incorporate human factors into the model via sequential estimations of a time-perturbed Hamiltonian approximation (Melnik, 1997a; Melnik, 1998a)

$$\tilde{\mathcal{H}} = \min_{\mathbf{u}(t) \in \mathcal{U}, t \leq \tau \leq t+\Delta t} \mathcal{H} \quad (4.40)$$

for each time subinterval  $t \leq \tau \leq t+\Delta t$  with  $t \in [0, T]$ . This formulation is more general than those resulted from conventional methodologies. Indeed, at each time subinterval the Hamiltonian is allowed to change based on the information accumulated up to that point to reflect dynamic changes in the environment in which the system operates. A new Hamiltonian estimation should be provided based on that information. In the context of ITS, Hamiltonian estimations can be obtained efficiently with the assistance of on-board equipment, including sensors, receivers, actuators, inter-vehicle communication systems, and on-board computers. Computational methodologies for solving the problem for each Hamiltonian estimation are known as they were developed for the numerical solution of HJB-based models (e.g., Ishii, 1987; Osher and Seithian, 1988; Falcone and Ferreti, 1994; Milner and Park, 1996). Finally, a general approach to the analysis of such models (obtained via a decision making process with limited information available) using tools of information theory and the Markov chain approximation method can be found in Melnik (1997a, 1998a, 2003d, 2008).

#### 5. Complex systems and coupled problems in mathematical modelling

In the previous sections we dealt with problems of control of complex systems where the integration of human factors into mathematical models becomes essential. In this sense, the considered problems are linked to the AI problems, given that learning is at the very heart of the problem of intelligence, both



biological and artificial. More generally, these problems have been subject of studies in cybernetics defined broadly, according to A.N. Kolmogorov, as a science concerned with the study of systems of any nature which are capable of receiving, storing, and processing information so as to use it for control. We term such systems complex when they consist of interacting parts such that as a whole they exhibit new properties compared to the properties of the individual parts.

First attempts to the analysis of such systems, extending the existing framework of dynamic systems, were given in Melnik (1996, 1997a, c, 1998a). This was developed further in Melnik (2003d) and in Melnik (2008). In Melnik (2003d), a general approach was proposed to both deterministic and stochastic dynamic problems in control theory that can be reduced to partial differential equations by using Bellman's approach. It was proposed to approximate the *original controlled dynamics* with a sequence of PDEs. By applying the Steklov–Poincaré operator technique the general form of equations in such a sequence was established. The derived models can describe the behaviours of systems beyond those governed by diffusion stochastic processes. In Melnik (2008), this idea was developed further and a general framework for the analysis of a connection between the training of artificial neural networks via the dynamics of Markov chains and the approximation of conservation law equations was proposed. The developed framework establishes an intrinsic link between microscopic and macroscopic models for evolution via the concept of perturbed generalized dynamic systems.

Such perturbed generalized dynamic systems interact with their environments, and due to a degree of uncertainty in this dynamic interaction, many associated problems require the development of approaches with a substantial reduction in a priori information required for their applications. Such situations are typical for most complex systems. In some cases, the analysis of such systems requires dealing with highly oscillatory functions acquired as a result of measurements. Already at the level of numerical integration such cases lead to non-trivial mathematical difficulties which were dealt with in Melnik and Melnik (1999) for univariable highly oscillatory functions and in Zotsenko and Melnik (2004), Melnik and Melnik (2001, 2002) for multi-variable situations.

Traditionally, systems with uncertainties are modelled with stochastic mathematical models, and examples of such situations can be readily found in a range of applications from physical systems (Kaupuzs et al., 2007, 2008), to biological systems and complex polymeric materials (Wei et al., 2005, 2009; Yang and Melnik, 2007, 2009), and to financial market (Zhang and Melnik, 2008), to name just a few. However, similar challenges can often be found in *coupled field theory* where we have to deal with intrinsic dynamic interactions between fields of different nature (Melnik, 1998c; Melnik and Roberts, 2002; Melnik and Povitsky, 2004, 2006; Melnik et al., 2008). From a physics point of view, starting from fundamental works of J.C. Maxwell and later A. Einstein, attempts have been made to unify four physical forces (electromagnetic, strong, weak, and gravitational) in one theory. While this discussion lies outside of the current paper, we note that a large subset of coupled field theory problems, dealing with physical and engineering applications, is often termed as multi-physics. The latter term, however, does not include many important classes of coupled problems describing complex systems from biology, chemistry, climate modelling, financial and other areas of applications of mathematical models (Melnik, 1998b; Mahapatra and Melnik, 2006a; Yang and Melnik, 2007). A more generic term for such problems that we have used is coupled multi-scale (Melnik and Roberts, 2004; Wei et al., 2005). Coupling may come from many different sources and here we provide examples of coupled systems from our own experience,

and therefore this brief survey of complex systems and associated with them coupled phenomena that follows is, as a consequence, non-exhaustive. Many important examples of coupled systems are provided by coupling of physical fields of different nature, e.g. mechanical and electric (Melnik, 1998c), leading to coupled dynamic problems of electro-elasticity. Earlier analysis of coupled problems of electro-elasticity led for the first time to the proof of well-posedness of the associated mathematical models, proposed by W. Voigt at the beginning of the 20th century, in the dynamic case (Melnik and Moskalkov, 1988; Melnik, 1991) followed by further generalization to the multi-dimensional case (Melnik and Moskalkov, 1991; Melnik, 2000b). Usually, only in the case of weakly coupled problems (e.g., under special type of boundary conditions) a conventional analysis may apply (Melnik and Melnik, 1998), while in most cases we have to resort to discrete approximations of coupled problems. Stability for associated discrete variationally based approximations for the one-dimensional case has been analysed in Melnik (1997b) and for the multi-dimensional case in Melnik and Zotsenko (2004). The result of these analyses was that the complete and rigorous derivation of the generalization of the classical Courant–Friedrichs–Lewy stability condition to the case of dynamic piezoelectricity was obtained.

Another typical example of coupling is provided by thermal and mechanical (Melnik, 2001a; Wang et al., 2006; Zhang et al., 2008), or in some cases, thermal, mechanical, and electric fields, leading to coupled problems of thermo-electroelasticity which in the general dynamic case were addressed in Melnik (2001b, 2003a).

In some cases, our coupled electro-mechanical or thermo-electromechanical systems may interact with fluid, acoustic, and/or other fields (Melnik, 2003b; Kamath et al., 2006).

Coupling may also come from the structure of the material where often it is necessary to account for its heterogeneous complex nature (Lassen et al., 2005) and/or its multi-component character (Kournytskyi et al., 2005) as is often the case for polymers and composites (Melnik, 2002, 2003c; Melnik et al., 2003b, 2005).

In addition to challenges brought by coupling, many such problems are strongly nonlinear as it is the case when we construct mathematical models for the description of such complex materials as shape memory alloys (SMA) (Melnik et al., 2000; Melnik and Roberts, 2003). In order to make the dynamic problem for SMA trackable in engineering applications, a dimensional reduction of the fully coupled dynamic three-dimensional model for SMA was for the first time proposed in Melnik et al. (2000). The reduced model was approximated by a system of differential-algebraic equations. This approach allowed to study both stress- and temperature-induced phase transformations and associated hysteresis phenomena in SMA structures in a unified manner (Melnik et al., 2001) and to extend the developed technique to the Cattaneo–Vernotte law for heat conduction (Strunin et al., 2001), following principles of extended thermodynamics, in the context of SMA (Melnik et al., 2002). In the multi-dimensional case, the developed approach for dynamic models of SMA and associated coupled multi-scale problems (Melnik and Roberts, 2004; Melnik and Povitsky, 2004) were put on a systematic basis via the centre-manifold theory and received its justification in a series of papers (Melnik and Roberts, 2003; Melnik et al., 2003a; Matus et al., 2004). Two-dimensional thermo-mechanical waves in SMA patches were first analysed in Wang and Melnik (2004) and in Wang and Melnik (2006a) where distributed mechanical loadings for patches of different sizes were studied. The results of such two-dimensional modelling were systematically compared with conventional one-dimensional models in Wang and Melnik (2006b), while in Wang and Melnik

(2006c) the effectiveness of the developed procedure was demonstrated for both the solution of a transient uncoupled thermoelastic problem, for which an analytical solution is known, as well as for the fully coupled problem in the two-dimensional case.

To make the dynamic model of SMA better amenable to engineering applications and to reduce further the computational cost, an empirical low-dimensional model was developed based on a combination of proper orthogonal decomposition and Galerkin projection (Wang and Melnik, 2005) which was applied to the modelling of martensitic phase transformations in ferro-electric/SMA patches (Wang and Melnik, 2007b). Another approach to dynamic models of SMA, based on the Chebyshev collocation method, was proposed in Wang and Melnik (2006d) where it was applied to the simulation of martensitic phase combinations in the two-dimensional case. More recently, in Wang and Melnik (2008a) the dynamics of such combinations during thermally induced transformations was studied in detail.

In Wang and Melnik (2007c), Chebyshev's collocation was applied to the analysis of SMA rods where the effect of internal friction was taken into account via Rayleigh's dissipation term. As expected, dissipation effects were enhanced by internal friction, while dispersion during wave propagations were induced by the presence of the interfacial energy term in the model. In Wang and Melnik (2007a) the method was applied to the analysis of macroscale damping effects induced by the first-order martensite phase transformations in a SMA rod. It was also shown that both mechanically and thermally induced phase transformations in SMA, as well as hysteresis effects, can efficiently be modelled by the finite volume method developed in Wang and Melnik (2007d) where it was applied in various one-dimensional (rods) and two-dimensional (patches) situations.

A unified variational framework was applied to the analysis of SMA-based thin films (Mahapatra and Melnik, 2006c) where phase nucleation phenomena under mechanical loading were accounted for. The approach combined the lattice-based kinetics involving the order variables and non-equilibrium thermodynamics (Mahapatra and Melnik, 2007a). The finite element-based approach was extended to the three-dimensional situations and multi-variant martensitic phase transformations (Mahapatra and Melnik, 2005a, b), developed into a general framework (Mahapatra and Melnik, 2006b), and exemplified with the analysis of cubic to tetragonal transformations (Mahapatra and Melnik, 2007b). Furthermore, a recently developed hybrid optimization methodology, combining the local and global search algorithms has proved to be a useful tool in studying the dynamics of phase combinations in SMA samples (Wang and Melnik, 2008b).

We conclude this brief survey of examples of complex systems for which coupling is essential by echoing R. Feynman's famous comments on the existence of "plenty of room at the bottom". Indeed, nanoscience and semiconductor technologies provide many instructive examples of complex systems. Many problems in this field can be reduced to the solution of an eigenvalue PDE problem for a system of coupled Schrodinger equations (Melnik and Mahapatra, 2007). While we can reduce such a problem to an algebraic eigenvalue problem, some non-trivial difficulties that require novel approaches may arise (Melnik, 2000a). Many problems in this field require accounting for non-local and non-equilibrium processes (Melnik and He, 2000a, b, c), and in some cases for transport processes that involve complex nonlinear phenomena due to light-matter interactions (Melnik and Rimshans, 2003; Radulovic et al., 2006). Analysis of complex nonlinear processes in heterostructures, coupled phenomena in low-dimensional semiconductor nanostructures (LDSN), and LDSN-based devices provide examples of new challenges that the coupled field theory faces in this area (Willatzen et al., 2003,

2004; Radulovic et al., 2004; Voon et al., 2005; Wen and Melnik, 2008a, b; Mahapatra et al., 2008; Sinha et al., 2008).

Although approximated by time-independent models on a number of occasions, many problems associated with complex systems and coupled phenomena are dynamic by their nature. The concept of perturbed generalized dynamic systems linked with the training of artificial neural networks via the dynamics of Markov chains (Melnik, 2008) could be useful in the analysis of such problems.

## 6. Concluding remarks

Efficiency of models describing the dynamics of complex systems often depends upon allowance made for human (e.g., operators/drivers) capabilities and/or limitations of these systems. As a result, the integration of human-related design and support activities in the engineering of complex systems become important topics of research as exemplified here by ITS. In this contribution we demonstrated how human factors can be effectively incorporated into the analysis and control of complex systems. As an example, the problem of ITS speed control, considered here as a decision making process with limited information available, was cast mathematically in the general framework of control problems and treated in the context of dynamically changing environments where control is coupled to human factors. We demonstrated that the problem can be reduced to a set of HJB equations where human factors are incorporated via estimations of the system Hamiltonian. These estimations can be obtained with the use of on-board equipment like sensors/receivers/actuators, in-vehicle communication devices, etc. The proposed methodology provides a way to integrate human factor into the solving process of the models for other complex dynamic systems.

## Acknowledgements

This work was originally inspired by discussions with the members of the Center for Industrial and Applied Mathematics at the University of South Australia, and the idea was developed further in discussions with the colleagues at the Mads Clausen Institute at the University of Southern Denmark. The author thank all of them for stimulating discussions and a creative multidisciplinary environment. The work has been completed in the M<sup>2</sup>NeT Laboratory (<http://www.m2netlab.wlu.ca>) and the author is grateful to the NSERC and CRC program for their support at the final stage of working on this paper.

## References

- Angelov, C., Melnik, R.V.N., Buur, J., 2003. The synergistic integration of mathematics, software engineering, and user-centred design: exploring new trends in education. *Future Generation Computer Systems* 19 (8), 1299–1307.
- Barthelemy, J.P., Bisdorff, R., Coppin, G., 2002. Human centered processes and decision support systems. *European Journal of Operational Research* 136 (2), 233–252.
- Butts, K.R., Sivashankar, N., Sun, J., 1999. Application of  $L_1$  optimal control to the engine idle speed control problem. *IEEE Transactions on Control Systems Technology* 7, 258–270.
- Carroll, J.M. (Ed.), 2003. *HCI Models, Theories, and Frameworks. Toward a Multidisciplinary Science*. Morgan Kaufmann Publishers.
- Endo, S., et al., 1999a. Simulation of speed control in acceleration mode of a heavy-duty vehicle. *JSAE Journal* 20, 81–86.
- Endo, S., et al., 1999b. A study on speed control law for automated driving of heavy-duty vehicles considering acceleration characteristics. *JSAE Journal* 20, 331–336.
- Endo, S., et al., 2000. A study on speed control law for automated driving of heavy-duty vehicles. *JSAE Journal* 21, 47–52.
- Falcone, M., Ferreti, R., 1994. Discrete time high-order schemes for viscosity solutions of HJB equations. *Numerical Mathematics* 67, 315–344.

- Fontaras, G., Samaras, Z., 2007. A quantitative analysis of the European Automakers voluntary commitment to reduce CO<sub>2</sub> emissions from new passenger cars based on independent experimental data. *Energy Policy* 35 (4), 2239–2248.
- Gollu, A., Variya, P., 1998. SmartAHS: a simulation framework for automated vehicles and highway systems. *Mathematical and Computer Modelling* 27, 103–128.
- Goodrich, M.A., Boer, E.R., 2000. Designing human-centered automation: trade-offs in collision avoidance system design. *IEEE Transactions on ITS* 1.
- Herty, M., Rascle, M., 2006. Coupling conditions for a class of second-order models for traffic flow. *SIAM Journal on Mathematical Analysis* 38 (2), 595–616.
- Howlett, P., 1990. An optimal strategy for the control of a train. *Journal of the Australian Mathematical Society B* 31, 457–471.
- Howlett, P., 1996. Optimal strategies for the control of a train. *Automatica* 32, 519–532.
- Howlett, P.G., 1996. Personal communication.
- Howlett, P.G., Pudney, P.J., 1995. *Energy-Efficient Train Control*. Springer, Berlin.
- Huai, Y., Melnik, R.V.N., Thogersen, P.B., 2003. Computational analysis of temperature rise phenomena in electric induction motors. *Applied Thermal Engineering* 23 (7), 779–795.
- Ishii, H., 1987. Perron's method for Hamilton–Jacobi equations. *Duke Mathematical Journal* 55, 369–384.
- Kamath, H., Willatzen, M., Melnik, R.V.N., 2006. Vibration of piezoelectric elements surrounded by fluid media. *Ultrasonics* 44 (1), 64–72.
- Kaupuzs, J., Melnik, R.V.N., Rimshans, J., 2007. Monte Carlo test of the Goldstone mode singularity in 3D XY model. *European Physical Journal B* 55 (4), 363–370.
- Kaupuzs, J., Melnik, R.V.N., Rimsans, J., 2008. Advanced Monte Carlo study of the Goldstone mode singularity in the 3D XY model. *Communications in Computational Physics* 4 (1), 124–134.
- Kessler, E., Knapen, E.G., 2006. Towards human-centred next term design: two case studies. *Journal of Systems and Software* 79 (3), 301–313.
- Kiencke, U., Nielsen, L., Sutton, R., et al., 2006. The impact of automatic control on recent developments in transportation and vehicle systems. *Annual Reviews in Control* 30 (1), 81–89.
- Kirk, D.E., 1970. *Optimal Control Theory*. Prentice-Hall, Englewood Cliffs, NJ.
- Kirlik, A., Miller, R.A., Jagacinski, R.J., 1993. Supervisory control in a dynamic and uncertain environment: a process model of skilled human–environment interaction. *IEEE Transactions on Systems, Man, and Cybernetics* 23, 929–951.
- Kolmanovskiy, I., van Nieuwstadt, M., Sun, J., 2000. Optimization of complex powertrain systems for fuel economy and emissions. *Nonlinear Analysis: RWA* 1, 205–221.
- Kournitskyi, T., Melnik, R.V.N., Gachkevich, A., 2005. Thermal behavior of absorbing and scattering glass media containing molecular water impurity. *International Journal of Thermal Sciences* 44 (2), 107–114.
- Kraiss, K.-F., Hamacher, N., 2001. Concepts of user centered automation. *Aerospace Science and Technology* 5 (8), 505–510.
- Lassen, B., Willatzen, M., Melnik, R., Lew Yan Voon, L.C., 2005. A general treatment of deformation effects in Hamiltonians for inhomogeneous crystalline materials. *Journal of Mathematical Physics* 46 (11), 112102.
- Lions, P.-L., 1982. *Generalized Solutions of Hamilton–Jacobi Equations*. Pitman, Boston.
- Mahapatra, D.R., Melnik, R., 2005a. A dynamic model for phase transformations in 3D samples of shape memory alloys. In: *Computational Science—ICCS 2005*, part 3. Book Series: Lecture Series in Computer Science, vol. 3516, pp. 25–32.
- Mahapatra, D.R., Melnik, R., 2005b. Three-dimensional mathematical models of phase transformation kinetics in shape memory alloys. *Dynamics of Continuous Discrete and Impulsive Systems Series B—Applications and Algorithms* 2, 557–562 (Sp. Iss. SI).
- Mahapatra, D.R., Melnik, R.V.N., 2006a. Modelling and analysis of collagen piezoelectricity in human cornea. *Dynamics of Continuous Discrete and Impulsive Systems Series A—Mathematical Analysis* 13 (Suppl. S), 377–384.
- Mahapatra, D.R., Melnik, R.V.N., 2006b. Finite element analysis of phase transformation dynamics in shape memory alloys with a consistent Landau–Ginzburg free energy model. *Mechanics of Advanced Materials and Structures* 13 (6), 443–455.
- Mahapatra, D.R., Melnik, R.V.N., 2006c. Numerical simulation of phase transformations in shape memory alloy thin films. In: *Computational Science—ICCS 2006*, part 2. Proceedings, Book Series: Lecture Notes in Computer Science, vol. 3992, pp. 114–121.
- Mahapatra, D.R., Melnik, R.V.N., 2007a. Finite element modelling and simulation of phase transformations in shape memory alloy thin films. *International Journal for Multiscale Computational Engineering* 5 (1), 65–71.
- Mahapatra, D.R., Melnik, R.V.N., 2007b. Finite element approach to modelling evolution of 3D shape memory materials. *Mathematics and Computers in Simulation* 76 (1–3), 141–148.
- Mahapatra, D.R., Sinha, N., Yeow, J.T.W., Melnik, R., 2008. Field emission from strained carbon nanotubes on cathode substrate. *Applied Surface Science* 255 (5), 1959–1966.
- Manzie, C., Watson, H., Halgamuge, S., 2007. Fuel economy improvements for urban driving: hybrid vs. intelligent vehicles. *Transportation Research Part C: Emerging Technologies* 15 (1), 1–16.
- Matus, P., Melnik, R.V.N., Wang, L., Rybak, I., 2004. Applications of fully conservative schemes in nonlinear thermoelasticity: modelling shape memory materials. *Mathematics and Computers in Simulation* 65 (4–5), 489–509.
- Mayer, F., Stahrea, J., 2006. Human-centred systems engineering (Editorial to a special issue). *Annual Reviews in Control* 30 (2), 193–195.
- Melnik, K.N., Melnik, R.V.N., 1999. Optimal-by-order quadrature formulae for fast oscillatory functions with inaccurately given a priori information. *Journal of Computational and Applied Mathematics* 110 (1), 45–72.
- Melnik, K.N., Melnik, R.V.N., 2001. Optimal cubature formulae and recovery of fast-oscillating functions from an interpolational class. *BIT Numerical Mathematics* 41 (4), 748–775.
- Melnik, K.N., Melnik, R.V.N., 2002. Optimal-by-accuracy and optimal-by-order cubature formulae in interpolational classes. *Journal of Computational and Applied Mathematics* 147 (1), 233–262.
- Melnik, R., Mahapatra, R., 2007. Coupled effects in quantum dot nanostructures with nonlinear strain and bridging modelling scales. *Computers and Structures* 85 (11–14), 698–711.
- Melnik, R.V.N., 1996. Non-conservation law equation in mathematical modelling: aspects of approximation. In: Yuen, W.Y.D., Broadbridge, P., Steiner, J.M. (Eds.), *Proceedings of the International Conference AEMC'96*, Sydney, Australia, ISBN 0-85825-653-3, pp. 423–430.
- Melnik, V.N., 1997a. On consistent regularities of control and value functions. *Numerical Functional Analysis and Optimization* 18, 401–426.
- Melnik, R.V.N., 1997b. The stability condition and energy estimate for nonstationary problems of coupled electroelasticity. *Mathematics and Mechanics of Solids* 2 (2), 153–180.
- Melnik, R.V.N., 1997c. A hierarchy of hyperbolic macrodynamic equations as a model for network training. In: *Proceedings of the IEEE International Symposium on Information Theory*, Ulm, Germany, p. 322.
- Melnik, R.V.N., 1998a. Dynamic system evolution and Markov chain approximation. *Discrete Dynamics in Nature and Society* 2, 7–39.
- Melnik, R.V.N., 1998b. Mathematical models for climate as a link between coupled physical processes and computational decoupling. *Engineering Simulation: An International Journal of Electrical, Electronic and Other Physical Systems* 15 (4), 509–544.
- Melnik, R.V.N., 1998c. Convergence of the operator-difference scheme to generalized solutions of a coupled field theory problem. *Journal of Difference Equations and Applications* 4 (2), 185–212.
- Melnik, R.V.N., 2000a. Topological analysis of eigenvalues in engineering computations. *Engineering Computations* 17 (4), 386–416.
- Melnik, R.V.N., 2000b. Generalised solutions, discrete models and energy estimates for a 2D problem of coupled field theory. *Applied Mathematics and Computation* 107 (1), 27–55.
- Melnik, R.V.N., 2001a. Discrete models of coupled dynamic thermoelasticity for stress-temperature formulations. *Applied Mathematics and Computation* 122 (1), 107–132.
- Melnik, R.V.N., 2001b. Computational analysis of coupled physical fields in piezothermoelastic media. *Computer Physics Communications* 142 (1–3), 231–237.
- Melnik, R.V.N., 2002. Models for coupled kinetics and heat transfer in processing polymeric materials with applications to biochemical engineering. *Modelling and Simulation in Materials Science and Engineering* 10 (3), 341–357.
- Melnik, R.V.N., 2003a. Modelling coupled dynamics: piezoelectric elements under changing temperature conditions. *International Communications in Heat and Mass Transfer* 30 (1), 83–92.
- Melnik, R.V.N., 2003b. Numerical analysis of dynamic characteristics of coupled piezoelectric systems in acoustic media. *Mathematics and Computers in Simulation* 61 (3–6), 497–507.
- Melnik, R.V.N., 2003c. Computationally efficient algorithms for modelling thermal degradation and spiking phenomena in polymeric materials. *Computers and Chemical Engineering* 27 (10), 1473–1484.
- Melnik, R.V.N., 2003d. Deterministic and stochastic dynamics with hyperbolic HJB-type equations. *Dynamics of Continuous Discrete and Impulsive Systems—Series A—Mathematical Analysis* 10 (1–3), 317–330.
- Melnik, R.V.N., 2008. Markov chain network training and conservation law approximations: linking microscopic and macroscopic models for evolution. *Applied Mathematics and Computation* 199 (1), 315–333.
- Melnik, R.V.N., He, H., 2000a. Quasi-hydrodynamic modelling and computer simulation of coupled thermo-electrical processes in semiconductors. *Mathematics and Computers in Simulation* 52 (3–4), 273–287.
- Melnik, R.V.N., He, H., 2000b. Modelling nonlocal processes in semiconductor devices with exponential difference schemes. *Journal of Engineering Mathematics* 38 (3), 233–263.
- Melnik, R.V.N., He, H., 2000c. Relaxation-time approximations of quasi-hydrodynamic type in semiconductor device modelling. *Modelling and Simulation in Materials Science and Engineering* 8 (2), 133–149.
- Melnik, R.V.N., Jenkins, D.R., 2002. On computational control of flow in airblast atomisers for pulmonary drug delivery. *International Journal of Pharmaceutics* 239 (1–2), 23–35.
- Melnik, R.V.N., Melnik, K.N., 1998. A note on the class of weakly coupled problems of non-stationary piezoelectricity. *Communications in Numerical Methods in Engineering* 14 (9), 839–847.
- Melnik, R.V.N., Melnik, K.N., 2000. Modelling dynamics of piezoelectric solids in the two-dimensional case. *Applied Mathematical Modelling* 24 (3), 147–163.
- Melnik, R.V.N., Povitsky, A., 2004. Wave phenomena in physics and engineering: new models, algorithms, and applications. *Mathematics and Computers in Simulation* 65 (4–5), 299–302.
- Melnik, R.V.N., Povitsky, A., 2006. A special issue on modelling coupled and transport phenomena in nanotechnology. *Journal of Computational and Theoretical Nanoscience* 3 (4), pp. i–ii.
- Melnik, R., Povitsky, A., Srivastava, D., 2008. Mathematical and Computational Models for Transport and Coupled Processes in Micro- and Nanotechnology. *Journal of Nanoscience and Nanotechnology* 8 (7), 3626–3627.
- Melnik, R.V.N., Rimshans, J., 2003. Numerical analysis of fast charge transport in optically sensitive semiconductors. *Dynamics of Continuous Discrete and*

- Impulsive Systems—Series B—Applications and Algorithms (Suppl. S), 102–107.
- Melnik, R.V.N., Roberts, A., 2004. Computational models for multi-scale coupled dynamic problems. *Future Generation Computer Systems* 20 (3), 453–464.
- Melnik, R.V.N., Roberts, A.J., 2001. Thermomechanical behaviour of thermoelectric SMA actuators. *Journal de Physique IV* 11 (PR8), 515–520.
- Melnik, R.V.N., Roberts, A.J., 2002. Computational models for materials with shape memory: towards systematic description of coupled phenomena. In: *Computational Science—ICCS 2002, part II. Book Series: Lecture Notes in Computer Science*, vol. 2330, pp. 490–499.
- Melnik, R.V.N., Roberts, A.J., 2003. Modelling nonlinear dynamics of shape-memory-alloys with approximate models of coupled thermoelasticity. *Zeitschrift für Angewandte Mathematik und Mechanik* 83 (2), 93–104.
- Melnik, R.V.N., Zotsenko, K.N., 2004. Mixed electroelastic waves and CFL stability conditions in computational piezoelectricity. *Applied Numerical Mathematics* 48 (1), 41–62.
- Melnik, R.V.N., Roberts, A.J., Thomas, K.A., 2000. Computing dynamics of copper-based SMA via centre manifold reduction of 3D models. *Computational Materials Science* 18 (3–4), 255–268.
- Melnik, R.V.N., Roberts, A.J., Thomas, K.A., 2001. Coupled thermomechanical dynamics of phase transitions in shape memory alloys and related hysteresis phenomena. *Mechanics Research Communications* 28 (6), 637–651.
- Melnik, R.V.N., Roberts, A.J., Thomas, K.A., 2002. Phase transitions in shape memory alloys with hyperbolic heat conduction and differential-algebraic models. *Computational Mechanics* 29 (1), 16–26.
- Melnik, R.V.N., Wang, L., Matus, P., Rybak, L., 2003a. Computational aspects of conservative difference schemes for shape memory alloys applications. In: *Computational Science and its Applications—ICCSA 2003, part 2. Proceedings, Book Series: Lecture Notes in Computer Science*, vol. 2668, pp. 791–800.
- Melnik, R.V.N., Uhlherr, A., Hodgkin, J., de Hoog, F., 2003b. Distance geometry algorithms in molecular modelling of polymer and composite systems. *Computers and Mathematics with Applications* 45 (1–3), 515–534.
- Melnik, R.V.N., Strunin, D.V., Roberts, A.J., 2005. Nonlinear analysis of rubber-based polymeric materials with thermal relaxation models. *Numerical Heat Transfer Part A—Applications* 47 (6), 549–569.
- Melnik, V.N., 1991. Theorems of existence and uniqueness of generalized solutions for one class of nonstationary problems of coupled electroelasticity. *Izvestiya Vysshikh Uchebnykh Zavedenii Matematika* 4, 24–32.
- Melnik, V.N., Moskalov, M.N., 1988. On the coupled nonstationary electrostatic oscillations of a piezoceramic cylinder with radial polarization. *USSR Computational Mathematics and Mathematical Physics* 28 (6), 109–110.
- Melnik, V.N., Moskalov, M.N., 1991. Difference schemes for and analysis of approximate solutions of 2D nonstationary problems in coupled electroelasticity. *Differential Equations* 27 (7), 860–867.
- Milner, F.A., Park, E.-J., 1996. Mixed finite-element methods for HJB-type equations. *IMA Journal of Numerical Analysis* 16, 399–412.
- Osher, S., Sethian, J.A., 1988. Fronts propagating with curvature-dependent speed: algorithms based on Hamilton–Jacobi formulations. *Journal of Computational Physics* 79, 12–49.
- Pontryagin, L.S., et al., 1986. *The Mathematical Theory of Optimal Processes*. Gordon & Breach.
- Pudney, P., Howlett, P., 1994. Optimal driving strategies for a train journey with speed limits. *Journal of the Australian Mathematical Society B* 36, 38–49.
- Qi, Y., Zhao, Y.Y., 2005. Energy-efficient trajectories of unmanned aerial vehicles flying through thermals. *Journal of Aerospace Engineering* 18 (2), 84–92.
- Radulovic, N., Willatzen, M., Melnik, R.V.N., 2004. Resonant tunneling heterostructure devices—dependencies on thickness and number of quantum wells. In: *Computational Science and Its Applications—ICCSA 2004, part 3. Book Series: Lecture Notes in Computer Science*, vol. 3045, pp. 817–826.
- Radulovic, N., Willatzen, M., Melnik, R.V.N., Lew Yan Voon, L., 2006. Influence of the metal contact size on the electron dynamics and transport inside the semiconductor heterostructure nanowire. *Journal of Computational and Theoretical Nanoscience* 3 (4), 551–559.
- Rouse, W.B., Edwards, S.L., Hammer, J.M., 1993. Modeling the dynamics of mental workload and human performance in complex systems. *IEEE Transactions on Systems, Man, and Cybernetics* 23, 1662–1671.
- Seto, Y., Inoue, H., 1999. Development of platoon driving in AHS. *JSAC Journal* 20, 93–99.
- Shahar, Y., et al., 2006. Distributed, intelligent, interactive visualization and exploration of time-oriented clinical data and their abstractions. *Artificial Intelligence in Medicine* 38 (2), 115–135.
- Sinha, N., Mahapatra, D.R., Sun, Y., Yeow, J.T.W., Melnik, R.V.N., Jaffray, D.A., 2008. Electromechanical interactions in a carbon nanotube based thin film field emitting diode. *Nanotechnology* 19 (2), 025701.
- Sivashankar, N., Sun, J., 1999. Development of model-based computer-aided engine control systems. *International Journal of Vehicle Design* 21, 325–343.
- Stotsky, A., Chien, C.-C., Ioannou, P., 1995. Robust platoon-stable controller design for autonomous intelligent vehicles. *Mathematical and Computer Modelling* 22, 287–303.
- Strunin, D.V., Melnik, R.V.N., Roberts, A.J., 2001. Coupled thermomechanical waves in hyperbolic thermoelasticity. *Journal of Thermal Stresses* 24 (2), 121–140.
- Sucharev, A., Timochov, A., Fedorov, V., 1989. *Optimization Methods*. Nauka.
- Voon, L.C.L.Y., Galeriu, C., Lassen, B., et al., 2005. Electronic structure of wurtzite quantum dots with cylindrical symmetry. *Applied Physics Letters* 87 (4), 041906.
- Wang, H.J., Dai, W.Z., Melnik, R., 2006. A finite difference method for studying thermal deformation in a double-layered thin film exposed to ultrashort pulsed lasers. *International Journal of Thermal Sciences* 45 (12), 1179–1196.
- Wang, L., Melnik, R.V.N., 2008c. Dynamic model of shape memory alloy oscillators for vibration frequency tuning and other applications, submitted for publication.
- Wang, L.X., Melnik, R., 2006a. Dynamics of shape memory alloys patches with mechanically induced transformations. *Discrete and Continuous Dynamical Systems* 15 (4), 1237–1252.
- Wang, L.X., Melnik, R.V.N., 2004. Thermomechanical waves in SMA patches under small mechanical loadings. In: *Computational Science—ICCS 2004, part 4. Proceedings, Book Series: Lecture Notes in Computer Science*, vol. 3039, pp. 645–652.
- Wang, L.X., Melnik, R.V.N., 2005. Simulation of nonlinear thermomechanical waves with an empirical low dimensional model. In: *Computational Science—ICCS 2005, part 1. Proceedings, Book Series: Lecture Notes in Computer Science*, vol. 3514, pp. 884–891.
- Wang, L.X., Melnik, R.V.N., 2006b. Two-dimensional analysis of shape memory alloys under small loadings. *International Journal for Multiscale Computational Engineering* 4 (2), 291–304.
- Wang, L.X., Melnik, R.V.N., 2006c. Differential-algebraic approach to coupled problems of dynamic thermoelasticity. *Applied Mathematics and Mechanics* 27 (9), 1185–1196.
- Wang, L.X., Melnik, R.V.N., 2006d. Mechanically induced phase combination in shape memory alloys by Chebyshev collocation methods. *Materials Science and Engineering A* 438, 427–430 (Sp. Iss.).
- Wang, L.X., Melnik, R.V.N., 2007a. Numerical model for vibration damping resulting from the first-order phase transformations. *Applied Mathematical Modelling* 31 (9), 2008–2018.
- Wang, L.X., Melnik, R.V.N., 2007b. Model reduction applied to square to rectangular martensitic transformations using proper orthogonal decomposition. *Applied Numerical Mathematics* 57 (5–7), 510–520.
- Wang, L.X., Melnik, R.V.N., 2007c. Thermo-mechanical wave propagations in shape memory alloy rod with phase transformations. *Mechanics of Advanced Materials and Structures* 14 (8), 665–676.
- Wang, L.X., Melnik, R.V.N., 2007d. Finite volume analysis of nonlinear thermo-mechanical dynamics of shape memory alloys. *Heat and Mass Transfer* 43 (6), 535–546.
- Wang, L.X., Melnik, R.V.N., 2008a. Modifying macroscale variant combinations in a two-dimensional structure using mechanical loadings during thermally induced transformation. *Materials Science and Engineering A* 481, 190–193 (Sp. Iss.).
- Wang, L.X., Melnik, R.V.N., 2008b. Simulation of phase combinations in shape memory alloys patches by hybrid optimization methods. *Applied Numerical Mathematics* 58 (4), 511–524.
- Wei, X., Melnik, R.V.N., Moreno-Hagelsieb, G., 2009. Nonlinear dynamics of cell cycles with stochastic mathematical models. *Journal of Biological Systems*, to appear.
- Wei, X.L., Melnik, R.V.N., Moreno-Hagelsieb, G., 2005. Modelling dynamics of genetic networks as a multiscale process. In: *Computational Science—ICCS 2005, part 3. Book Series: Lecture Notes in Computer Science*, vol. 3516, pp. 134–138.
- Wen, B., Melnik, R.V.N., 2008a. First principles molecular dynamics study of CdS nanostructure temperature-dependent phase stability. *Applied Physics Letters* 92 (26), 261911.
- Wen, B., Melnik, R.V.N., 2008b. Relative stability of nanosized wurtzite and graphitic ZnO from density functional theory. *Chemical Physics Letters* 466 (1–3), 84–87.
- Willatzen, M., Melnik, R.V.N., Galeriu, C., Lew Yan Voon, L., 2003. Finite element analysis of nanowire superlattice structures. In: *Computational Science and Its Applications—ICCSA 2003, part 2. Book Series: Lecture Notes in Computer Science*, vol. 2668, pp. 755–763.
- Willatzen, M., Melnik, R.V.N., Galeriu, C., Lew Yan Voon, L., 2004. Quantum confinement phenomena in nanowire superlattice structures. *Mathematics and Computers in Simulation* 65 (4–5), 385–397.
- Wren, C.R., Minnen, D.C., Rao, S.G., 2006. Similarity-based analysis for large networks of ultra-low resolution sensors. *Pattern Recognition* 39 (10), 1918–1931.
- Wu, Z., Melnik, R.V.N., Borup, F., 2006. Model-based analysis and simulation of regenerative heat wheel. *Energy and Buildings* 38 (5), 502–514.
- Wu, Z., Melnik, R.V.N., Borup, F., 2007. Model-based analysis and simulation of airflow control systems of ventilation units in building environments. *Building and Environment* 42 (1), 203–217.
- Xu, M., Melnik, R.V.N., Borup, U., 2004. Modeling anti-islanding protection devices for photovoltaic systems. *Renewable Energy* 29 (15), 2195–2216.
- Yang, X.D., Melnik, R.V.N., 2007. Effect of internal viscosity on Brownian dynamics of DNA molecules in shear flow. *Computational Biology and Chemistry* 31 (2), 110–114.
- Yang, X.D., Melnik, R.V.N., 2009. Effect of internal viscosity of polymeric fluids under strong extensional flows. *Chinese Journal of Polymer Science* 27 (1), 1–5.
- Zhang, D., Melnik, R.V.N., 2008. First passage time for multivariate jump-diffusion processes in finance and other areas of applications. *Applied Stochastic Models in Business and Industry*, in press, doi:10.1002/asmb.745.
- Zhang, S.Y., Dai, W.Z., Wang, H.J., et al., 2008. A finite difference method for studying thermal deformation in a 3D thin film exposed to ultrashort pulsed lasers. *International Journal of Heat and Mass Transfer* 51 (7–8), 1979–1995.
- Zhuan, X., Xia, X., 2006. Cruise control scheduling of heavy haul trains. *IEEE Transactions on Control Systems Technology* 14 (4), 757–766.
- Zotsenko, K.N., Melnik, R.V.N., 2004. Optimal minimax algorithm for integrating fast oscillatory functions in two dimensions. *Engineering Computations* 21 (7–8), 834–847.