

# A Variational Approach For A Slow Motion Of Aerosol Particles In The Atmospheric Fluid

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## 1. Introduction

There are the two broad categories of approaches where methods of the contemporary mathematical theory of optimization can be used for analyzing thermodynamic systems. In the first category, one wants to *optimize* these systems by changing some external parameters (decisions or controls). In this case both extremal and non-extremal solutions pertain to real physical situations, and the governing equations describe the dynamical changes of the internal state and controls imposed through the system boundaries. This first category includes studies which seek in-principle limits to the operation of thermodynamic processes and studies which seek to improve existing engineering systems. In the second approach, one wants to predict the system behavior (usually irreversible) under prescribed external conditions and therefore seeks to derive its governing equations from certain variational or extremum principles. It may be said that in this case the extremal control is set by nature rather than by man.

In this paper we discuss the second approach in the context of motion of aerosol particles in an atmospheric viscous fluid (Davis 1966). Consider an aerosol particle treated as a macroscopic body moving in the atmosphere, where the presence of the friction phenomena results in the appearance of certain additional frictional forces. Can we describe the system in terms of a variational principle taking into account dissipation? Despite of many negative opinions regarding this question (e.g. Milikan 1929; Yourgrau and Mandelstam 1968; Ray 1979) various kinetic potentials generalizing the classical, reversible Lagrangian

$$L = m\mathbf{u}^2/2 - V(\mathbf{x}), \quad (1)$$

have been advanced (Bateman 1929; Denman and Buch 1962; Kiehn 1975; Sieniutycz 1976; Vujanovic and Jones 1988; Vujanovic 1992). Before we enunciate reasons for their limited success, let us characterize the energy terms appearing in Eq (1). For a particle suspended in the fluid, mass  $m$  should be understood as an effective mass defined as the sum of the actual mass of the particle,  $m_p$ , and the virtual mass of the accreted fluid,  $m_f$ . The hydrodynamic considerations yield  $m_f = (1/2)\rho_f v_p$  i.e. the virtual mass is one half of the fluid mass contained in the volume occupied by the particle. The particle volume  $v_p$  is also the parameter of potential energy  $V$  because the potential energy of the particle-fluid system equals  $(\rho_p - \rho_f)v_p \mathbf{g} \cdot \mathbf{x}$ , i.e. it contains the Archimedes term related to the buoyancy force. Thus the explicit form of the particle Lagrangian is

$$L = (\rho_p + \rho_f/2)_p \mathbf{u}^2/2 - (\rho_p - \rho_f)_p \mathbf{g} \cdot \mathbf{x} \quad (2)$$

where the product of the (constant) gravitational field strength and radius vector  $\mathbf{g} \cdot \mathbf{x}$  represents the potential energy per unit mass. However Eqs. (1) and (2) refer to non-dissipative motions only, i.e. they do not predict frictional (Stokes) forces in the system.

To date, kinetic potentials generalizing (1) or (2) to irreversible motions have had very limited success even for simple systems. One such method, originated by Bateman (1929), uses a modified, time dependent Lagrangian  $L_\tau = L \exp(t/\tau)$ , where  $\tau$  is a time constant describing an interaction of the body with the fluid and  $L$  is the classical (Hamilton's) kinetic potential. The reader can verify that for  $L = m\mathbf{u}^2/2 - \mathbf{l}(\mathbf{x})$ , the nonautonomous Lagrangian

$$L_\tau = L \exp(t/\tau) \quad (3)$$

leads to the proper "frictional" force  $\tau \partial L / \partial \mathbf{u} = m\mathbf{u}/\tau$  in the equation of motion corresponding to laminar friction.

However the physical interpretation of the related Hamiltonian in energy terms is awkward since the nonautonomous Lagrangian (3) leads to the Hamiltonian  $H_\tau$

$$H_\tau = \frac{\partial L_\tau}{\partial \mathbf{u}} \cdot \mathbf{u} - L_\tau = \left( \frac{\partial L}{\partial \mathbf{u}} \cdot \mathbf{u} - L \right) \exp(t/\tau) = E \exp(t/\tau) \quad (4)$$

which is not a constant of the irreversible motion. On the other hand the standard energy  $E$  understood as the Legendre transform of reversible  $L$  is the constant of the reversible motion. The violation of the constancy property for the "irreversible" Hamiltonian  $H_\tau$  poses a serious physical problem since the autonomous nature of the dynamical system involved dictates that its Hamiltonian should be a constant of motion.

Below we explore a different modification by making an assumption that the Lagrangian of the irreversible motion  $L_\tau$  is an action dependent rather than time dependent quantity, so that action  $A$  or action variable  $x_0 \equiv -A$  should explicitly appear in  $L_\tau$ . Since in this formulation  $L_\tau$  does not contain explicitly time  $t$ , the irreversibility is no longer associated with the time dependent properties of the Lagrangian  $L_\tau$ . Speaking in more concrete terms, the proposed approach is accomplished by introducing an extra additive term  $\tau^{-1}x_0$  into Lagrangian  $L_\tau$ . This assumption allows to secure the constancy of the autonomous Hamiltonian  $H_\tau$ , and has some other virtues that are discussed in the further text. We shall also stress that with this approach one shall be able to discuss the energy conservation and achieve a satisfactory set of equations of motion. An extension of this model will enable one to discuss the Brownian diffusion in the concentrated aerosols, and to formulate an extended variational formulation for the case of concentrated suspensions governed by behavior of the chemical potential.

## 2. New Formulation involving the Maximum Principle

The maximum principle (Pontryagin *at al* 1962) reduces the global problem of the maximizing the functional to the problem of the maximizing the function  $H$  at each instant. In the cases when an analytical solution is impossible or difficult, this method

also allows to organize an approximating numerical scheme using a large but finite number of the time instants which give a discrete approximation for the optimal path and the corresponding optimal control.

The Euler equations of variational calculus can be obtained by investigating an extremum of the action objective  $x_0(t^f)$ . By definition, the variable  $x_0$  is the negative action variable, such that  $x_0(t^f) = -A(t^f)$ . Writing the objective in the form of the integral

$$x_0(t^f) = x_0(t^i) + \int_{t^i}^{t^f} f_0(x_0, \mathbf{x}, \mathbf{u}, t) dt \equiv -A(t^f) \quad (5)$$

we consider the necessary optimality conditions for the maximum of  $x_0(t^f)$  under the simple differential constraints

$$d\mathbf{x}/dt = \mathbf{u} \quad (6)$$

for the  $n$ -component vector  $\mathbf{x} = (x_1, x_2, \dots, x_n)$ , the subset of the action-including  $n + 1$  dimensional vector  $\mathbf{X} = (x_0, x_1, x_2, \dots, x_n)$ . Here  $\dim \mathbf{u} = \dim \mathbf{x} = n$ . From Eq. (5) one has in terms of  $\mathbf{x}$  and  $x_0$  rather than  $\mathbf{X}$

$$\frac{dx_0}{dt} = f_0(x_0, \mathbf{x}, \mathbf{u}, t) \quad (7)$$

For the problems of analytical mechanics, the negative of  $f_0$ , designated as  $L(\mathbf{x}, \mathbf{u}, t)$ , is the Hamilton's kinetic potential  $L$  equal (nonrelativistically) to the difference between the kinetic and potential energies. In the classical case  $L$  is defined by Eqs. (1) and (2), in the irreversible case we use an action-dependent  $L$ , Eq. (15) below. Classically, however, the action  $A$  and kinetic potential  $L$  depend only on the coordinates of the original state vector  $\mathbf{x} = (x_1, \dots, x_n)$  which does not contain the variable  $x_0$ . This results in the constancy of the action adjoint  $z_0 = 1$  along the path both in the classical (reversible) model and in extended time-dependent models described in Sec.1.

The Hamiltonian of the considered process has the structure

$$H = z_0 f_0 + z_1 u_1 + \dots z_n u_n. \quad (8)$$

and the action extremum conditions are contained in the canonical set which is

$$\frac{dx_v}{dt} = \frac{\partial H}{\partial z_v}, \quad v=0, 1, 2 \dots n \quad (9)$$

$$\frac{dz_v}{dt} = -\frac{\partial H}{\partial x_v}, \quad v=0, 1, 2 \dots n \quad (10)$$

$$\frac{dH}{dt} = \frac{\partial H}{\partial t} \quad (11)$$

and

$$z_t + \max_{\mathbf{u}} H(x_0, \mathbf{x}, z_0, \mathbf{z}, t, \mathbf{u}) = 0. \quad (12)$$

( $n$  is the dimensionality of the state space without the action coordinate). Equation (9) reproduces the state equations (5) and (7), Eq. (10) are equations of motion, and Eq. (11) describes the dynamical behavior of extremum Hamiltonian. The equation (12) is of Hamilton-Jacobi-Bellman type, and it means that an optimal control must maximize  $H$  at each instant of time in the interval  $t' \leq t \leq t''$  (Pontryagin's Maximum Principle).

In accordance with the Pontryagin's Maximum Principle, the maximum of the variable  $x_0(t^f) = -A(t^f)$  or the minimum of final action  $A(t^f)$  requires the stationarity condition for the Hamiltonian with respect to controls  $u_k$ . This requirement leads to the relations

$$z_k = -\partial f_0 / \partial u_k = \partial L / \partial u_k, \quad k = 1, \dots, n, \quad (13)$$

which define generalized momenta  $z_k$ , also called state adjoints.

Equations (8) and (13) and the satisfaction of the condition  $z_0 = 1$  in a reversible process prove that, in the case of a nondissipative motion, the extremum Hamiltonian  $H$  is the energy of the process satisfying the standard definition  $E = \mathbf{z} \cdot \mathbf{u} - L$ . For autonomous systems, where  $L = f_0$  does not contain the time explicitly,  $H$  is a constant along the optimal arc. We associate the motion of such a system with "conservative" or "reversible" behavior. Yet, as already said, neither energy  $E$  (or the time-dependent Hamiltonian  $H_\tau$ , Eq. (4)) nor the generalized momenta are constants in the irreversible model described by Es. (3) and (4).

On the other hand, when the responsibility to handle the irreversibility is taken over by action variable of Eq. (5) the definitions of generalized momenta (13) will be affected by the non-constant variable  $z_0$ . Indeed, in this case, we obtain instead of Eq. (13)

$$z_k = -z_0 \partial f_0 / \partial u_k = z_0 \partial L / \partial u_k, \quad (14)$$

and thus from (8) and (10)

$$\frac{d}{dt} (z_0 \partial L / \partial \dot{\mathbf{x}}) = z_0 \frac{\partial L}{\partial \mathbf{x}} \quad (15)$$

These results show that the generalized momenta of the irreversible process are  $z_0 \partial L / \partial \mathbf{u}$  rather than  $\partial L / \partial \mathbf{u}$ . The consequence of this property are frictional forces discussed in Sec.3. Only for the "reversible" momenta (13) the canonical equations (10) yield

$$\frac{d}{dt} (\partial L / \partial \dot{\mathbf{x}}) = \frac{\partial L}{\partial \mathbf{x}} \quad v = 1, 2, \dots, n \quad (16)$$

which are the well known Euler equations of the variational calculus written in a vector form. They are usually suitable for describing the reversible microscopic motion of elementary particles or the frictionless motion of macroscopic bodies in inviscid media or in a vacuum.

### 3. Irreversible motions

Consider now a macroscopic body moving in a (resting) viscous fluid where friction phenomena result in additional frictional forces. We should keep in mind that the physical interpretation of the Hamiltonian (4) in energy terms is awkward and not admissible from the physical viewpoint since the system is autonomous and the Hamiltonian  $H_\tau$  is not a constant of the motion.

We thus explore a different modification by introducing an extra additive term into  $f_0$  of the form  $\tau^{-1}x_0$  so that the action variable  $x_0$  will explicitly appear in  $f_0$ . Thus,

$$f_0 = -\{m\mathbf{u}^2/2 - V(\mathbf{x}) + \tau^{-1}x_0\} \quad (17)$$

The Hamiltonian  $H = \mathbf{z} \cdot \mathbf{u} + z_0 f_0$  now contains the variable adjoint  $z_0$ . The canonical Eq. (9) recovers the state equations (6) and (7), whereas the canonical Eq. (10) yields the dynamical equations

$$\frac{d\mathbf{z}}{dt} = -\frac{\partial H}{\partial \mathbf{x}} = -z_0 \frac{\partial V}{\partial \mathbf{x}}, \quad (18)$$

$$\frac{dz_0}{dt} = -\frac{\partial H}{\partial x_0} = z_0 \tau^{-1}, \quad (19)$$

whereas the condition of the stationary extremum of the Hamiltonian with respect to the control  $\mathbf{u}$ , Eq. (12), yields  $\mathbf{z} = -z_0 \partial f_0 / \partial \mathbf{u} = -z_0 \partial L / \partial \mathbf{u}$  which (again) shows that the generalized momenta of the irreversible process are  $z_0 \partial L / \partial \mathbf{u}$  rather than  $\partial L / \partial \mathbf{u}$ . Using the transversality condition  $z_0(t^f) = 1$ , we can evaluate the time behavior of  $z_0$ . On the basis of Eq. (19), we see that  $z_0$  is exponential in time, e.g.,  $z_0(t) = \exp(t/\tau)$ . In fact, the consideration of the boundary condition yields  $\mathbf{z} = \exp[(t - t^f)/\tau] \partial L / \partial \mathbf{u}$ , which explains the limited success of the modified kinetic potential  $L \exp(t/\tau)$ , mentioned earlier. Incidentally, both modifications lead to the same, or proportional, generalized momenta  $\mathbf{z}$ . Substituting  $\mathbf{z} = \exp[(t - t^f)/\tau] \partial L / \partial \mathbf{u}$  into Eq. (18) and then using (19) yields the simplest possible equation of motion with a friction term

$$\frac{d}{dt} \left( \frac{\partial L}{\partial \dot{\mathbf{x}}} \right) + \tau^{-1} \frac{\partial L}{\partial \dot{\mathbf{x}}} - \frac{\partial L}{\partial \mathbf{x}} = 0 \quad (20)$$

In terms of the classical momenta  $\partial L / \partial \dot{\mathbf{x}} = m \mathbf{dx}/dt = m\mathbf{u}$  and the potential energy  $V$

$$\frac{d}{dt} (m\dot{\mathbf{x}}) + \tau^{-1} m\dot{\mathbf{x}} = -\frac{\partial V}{\partial \mathbf{x}} \quad (21)$$

The case  $\tau^{-1} = 3\pi\nu\delta/m$  corresponds with the Stokes frictional force exerted by a spherical body of diameter  $\delta$  and (effective) mass  $m$ , moving in a fluid with dynamic viscosity  $\nu$ .

#### 4. Conserved Hamiltonian

Consider the Hamiltonian  $H = \mathbf{z} \cdot \mathbf{u} + z_0 f_0$  along the extremal trajectory. It is defined on the space  $(\mathbf{X}, \mathbf{Z})$  or  $(\mathbf{x}, x_0, \mathbf{z}, z_0)$ . The extremum Hamiltonian  $H^e(\mathbf{x}, x_0, \mathbf{z}, z_0)$  is obtained by substituting  $\mathbf{u}$  expressed in terms of the  $(\mathbf{x}, x_0, \mathbf{z}, z_0)$  into  $H$ . Since for our model  $\mathbf{z} = -z_0 \partial f_0 / \partial \mathbf{u} = z_0 \partial L / \partial \mathbf{u} = z_0 m \mathbf{u}$  and hence  $\mathbf{u} = \mathbf{z} / (m z_0)$ , we obtain

$$H^e(\mathbf{x}, x_0, \mathbf{z}, z_0) = \frac{\mathbf{z}^2}{2mz_0} + z_0 V(\mathbf{x}) - \frac{z_0 x_0}{\tau} = \exp\left(\frac{t-t^f}{\tau}\right) \left( \frac{m\mathbf{u}^2}{2} + V(\mathbf{x}) - \frac{x_0}{\tau} \right) \quad (22)$$

This Hamiltonian is the constant of an "irreversible" (damped) motion governed by the canonical equations written for  $H^e$  in the space of the natural variables  $(\mathbf{x}, x_0, \mathbf{z}, z_0)$ . These canonical equations are equivalent with dynamical equations (18) – (20) describing for  $H = H^e$  the time evolution of the generalized momenta and the velocities expressed in terms of the canonical variables

$$\frac{d\mathbf{x}}{dt} = -\frac{\mathbf{z}}{mz_0} \quad (23)$$

and

$$\frac{dx_0}{dt} = -\frac{\mathbf{z}^2}{2mz_0^2} + V(\mathbf{x}) - \frac{x_0}{\tau} \quad (24)$$

Thus we have found a variational formulation for our irreversible system. The price for taking the irreversibility into account is not low. First, the usual space of the mechanical variables  $(\mathbf{x}, \mathbf{z})$  had to be replaced by the enlarged space  $(\mathbf{x}, x_0, \mathbf{z}, z_0)$ . Second, the extremum Hamiltonian is not the classical energy.

However,  $H^e$  is a constant of motion of the irreversible canonical equations (18) and (19) or (23) and (24). Also, any generalized momentum  $z_i$  is the constant of motion when the external field  $V(\mathbf{x})$  vanishes or is independent of the coordinate  $x_i$ . This proves that the (autonomous) irreversible process is in fact conservative if the macroscopic energy and momenta are properly defined. It only behaves like nonconservative when we are using the standard definitions of the energy and momenta formulated for reversible processes. Furthermore, in the limiting case of infinite  $\tau$ , the Hamiltonian becomes the classical energy of the body. This limit corresponds to the vanishing frequency  $\tau^{-1}$  of collisions between the body and the molecules of the reservoir. In this limit, the adjoint variables  $\mathbf{z}$  become the usual, classical momenta. Hence the correspondence of the formalism with the frictionless case is assured. In conclusion, variational treatments may be formulated for quite general irreversible dynamical systems. These treatments require extended definitions of the energy and

momenta and give an explicit role to the individual actions of the bodies involved. Some further details can be obtained for complex systems which require a vector of actions (Sieniutycz 1990).

An extension of this model based on an earlier work (Sieniutycz 1984) may deal with concentrated suspensions where the potential energy term should be properly generalized so as to include the specific chemical potential as a statistical measure of the internal energy of the particle which moves along a Lagrangian trajectory. This will enable one to discuss the Brownian diffusion in the concentrated aerosols, and to formulate an extended variational formulation for the case of concentrated suspensions governed by behavior of the chemical potential.

## 5. Concluding remarks

The variational model proposed in this work has some essential virtues in comparison with time dependent models originated from nonconservative (Bateman) Lagrangians which involve explicitly time and restrict the researcher to attribute the irreversibility to the non-conservative properties of the Hamiltonian  $H_t$ . In the action model proposed here the momentum variable  $p_0$  associated with action  $A(t^f)$  or action coordinate  $x_0(t) = -A(t)$  is essential. While the momentum-type variable  $p_0$  is constant in both reversible models and models based on nonconservative (e.g. Bateman) Lagrangians, in the action-involving models  $p_0$  grows monotonically (here: exponentially) in time, thus exhibiting the property of an evolution coordinate, similar to the entropy of the isolated thermodynamic system. As contrasted with the nonconservative model, the time adjoint  $z_t$  of the present model remains constant in time, hence the generalized (action involving) energy of the system  $H^e$

$$H^e = \exp\left(\frac{t-t^f}{\tau}\right)\left(\frac{m\mathbf{u}^2}{2} + V(\mathbf{x}) - \frac{x_0}{\tau}\right) \quad (25)$$

is also the constant of the irreversible motion of the system. In the case when the time between collisions tends to infinity or the parameter describing the frequency of collisions  $\tau^{-1}$  tends to zero the Hamiltonian obtained here approaches the classical reversible Hamiltonian, corresponding with the classical energy

$$H^e = \frac{m\mathbf{u}^2}{2} + V(\mathbf{x}) \quad (26)$$

The Hamiltonian function (25) obtained via optimization can thus be seen as extension of the standard energy for imperfect systems with friction. Setting to zero of the total time derivative of the conserved Hamiltonian (25) leads to the conclusion that the classical reversible energy (26) decreases in the irreversible process in time in accordance with the formula

$$\frac{d}{dt}\left(\frac{m\mathbf{u}^2}{2} + V(\mathbf{x})\right) = -\frac{(1/2)m\mathbf{u}^2 + V(\mathbf{x})}{\tau} \quad (27)$$

The right hand side of this equation with an opposite sign defines also the rate of growth of the classical internal energy of the system caused by the friction phenomena.

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