MACRODISPERSION AND DISPERSIVE TRANSPORT BY UNSTEADY RIVER FLOW UNDER UNCERTAIN CONDITIONS

M.L. Kavvas and L.Liang

UCD J.Amorocho Hydraulics Laboratory

University of California, Davis, CA 95616, USA

Uncertainties existing in the numerical simulations of river flow and solute transport

1. Spatial and temporal variability in flow conditions

    -geometry (channel width, elevation, length, roughness)

    -initial and boundary conditions of flow field

    -net lateral inflow/outflow from/to surrounding landscape as sinks/sources

2. Spatial and temporal variability in solute conditions

    -chemical and biological reaction rates

    -solute concentration in the point and non-point sinks/sources

3. Field measurement

    -measurement errors

    -limited Sampling

Modeling the open channel flow within the framework of uncertain parameters

1. Generate 700 realizations of the uncertain flow parameters, such as channel width, bed slope, lateral inflow, and Manning's roughness, used in the one-dimensional open channel flow simulation.

   All the uncertain parameters are assumed to be normal distributions or log-normal distributions. Their CVs (absolute value of the ratio of the standard deviation to the mean) are set between 0.25 to 1.0 based on literature review.

2. Simulate the uncertain open channel flow fields by Monte Carlo method. One realization of the flow field is obtained by the numerical solution of de Saint Venant's equation with a randomly generated set of flow parameter values. By randomly generating 700 sets of parameter values and solving de Saint Venant's equation 700 times with each of these generated sets of parameter values, 700 realizations of the open channel flow field are obtained.

de Saint Venant's Equations

$$\partial Q/\partial x + \partial A/\partial t = q_l$$

$$\frac{\partial}{\partial t}(Q) + \frac{\partial}{\partial x}\left(\frac{Q^2}{A}\right) + gA\frac{\partial h}{\partial x} + gA\left(S_f - S_0\right) = 0$$

Q is the flow discharge
A is the rectangular cross-sectional area
q_l is the distributed lateral inflow or outflow per unit length of channel resulting from overland flow and seepage
h is the flow depth; g is the gravitational acceleration
S_0 is the slope of the channel bed
S_f is the friction slope,

$$S_f = Q|Q|/K^2$$

K is conveyance,

$$K = (1.0/n) * A * R^{2/3};$$

n is Manning's roughness coefficient
R is hydraulic radius of the cross section

In the stochastic flow model, the major uncertainty associates with

the geometric and physical parameters and flow sources (lateral inflow/outflow).

In nature, at the local scale of a river cross-section

these geometric parameters, such as river width, bed slope, and Manning's coefficient

used in the stochastic flow model,

are spatially random,

while the lateral inflow/outflow is spatially and temporally random.

Accordingly, the flow equations employing these random parameters are taken as

Stochastic Partial Differential Equations (SPDEs)

at the local scale of a river cross-section.

The flow variables, flow depth and discharge, that are generated from these SPDEs,

are obviously spatiotemporal stochastic functions. `

Channel lateral inflow is generated as a spatiotemporal random field with normal distribution. This field is defined by the form;

$$F(x,t;r) = \sigma\varepsilon(x,t) + m$$

where F is a random field; x is the spatial location; t is the time; r is the index of realizations; σ is the standard deviation of the parameter; ε is a delta-correlated random function which is normally distributed with mean 0, variance 1 and standard deviation 1; and m is the mean of the parameter.

Considered as geometric properties, channel bed slope and channel width are taken spatially random with normal distribution. Manning's resistance coefficient is taken spatially random with lognormal distribution, which can also be transformed into a normal distribution. They can then be defined respectively in the form;

$$F(x;r) = \sigma\varepsilon(x) + m$$

Using one realization of the randomly generated parameters as input, the governing equations are numerically solved to predict the realizations of the random flow depth h(x, t; 1) and discharge Q(x, t; 1). The random velocity v(x, t; 1), which has fundamental effect on stochastic solute transport, is computed by using the values of h(x, t; 1) and Q(x, t; 1).

This step is repeated numerous times (r = 1,2,3,…) to obtain ensembles for the dependent variables

h(x, t;), Q(x, t;) and v(x, t;).

These ensembles are analyzed to estimate the means and variances

of the dependent variables

h(x, t;), Q(x, t;) and v(x, t;).

These ensembles are also used to compute the covariance integral terms, including the time-space varying macrodispersion coefficient, as coefficients in the ensemble-averaged solute transport equation.

A hypothetical transport problem is posed on a 20-km river reach that has uncertainties in its physical properties.

In this problem the lateral inputs and channel physical parameters, such as lateral inflow, lateral solute concentration, channel bed slope, roughness coefficient, channel width, and reaction rate, are assumed to be random.

In order to determine how these stochastic parameters affect the solute transport process, three cases are studied. Their statistical values, such as the mean and CV (absolute value of the ratio of the standard deviation to the mean) for three cases, are given in the next table.

Parameters	Mean	CV			Distribution
		Case 1	Case 2	Case 3	
Lateral inflow $\mathbf{q_l}$ (m^2/s)	0.006	1.0	0.5	1.0	Normal
Lateral solute concentration $\mathbf{c_l}$ (mg/m^3)	9.0	1.0	0.5	1.0	Normal
Channel bed slope $\mathbf{S_0}$	0.001	0.5	0.25	0.5	Normal
Manning's roughness **n**	0.037	0.25	.125	0.25	Log normal
Channel width **B** (m)	8.0	0.25	.125	0.25	Normal
Diffusion at the local scale **D** (m^2/s)	0	0	0	0	N/A
Reaction rate **K**(1/day)	1.0	0	0	1.0	Normal
Point source of solute **S** (mg/s/m)	.00025	0	0	1.0	Normal

The flow rate at the upstream boundary is assumed to be a delta-correlated random value, at statistical equilibrium in time, and normally distributed.

The mean flow rate at the upstream boundary equals $5m^3/s$ and its CV equals 0.25.

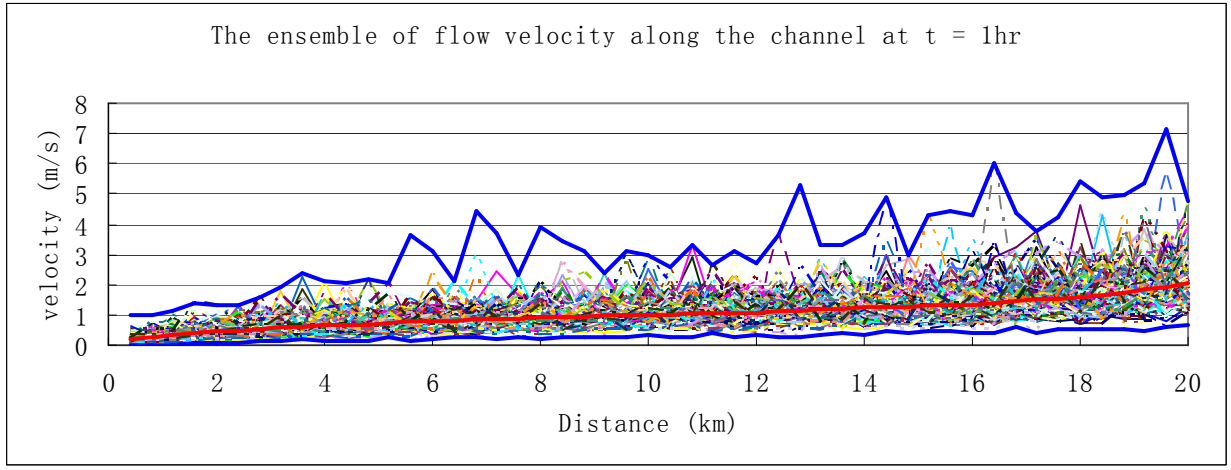
The downstream boundary condition is taken as normal flow, so the discharge and depth at the downstream cross-section satisfy the function,

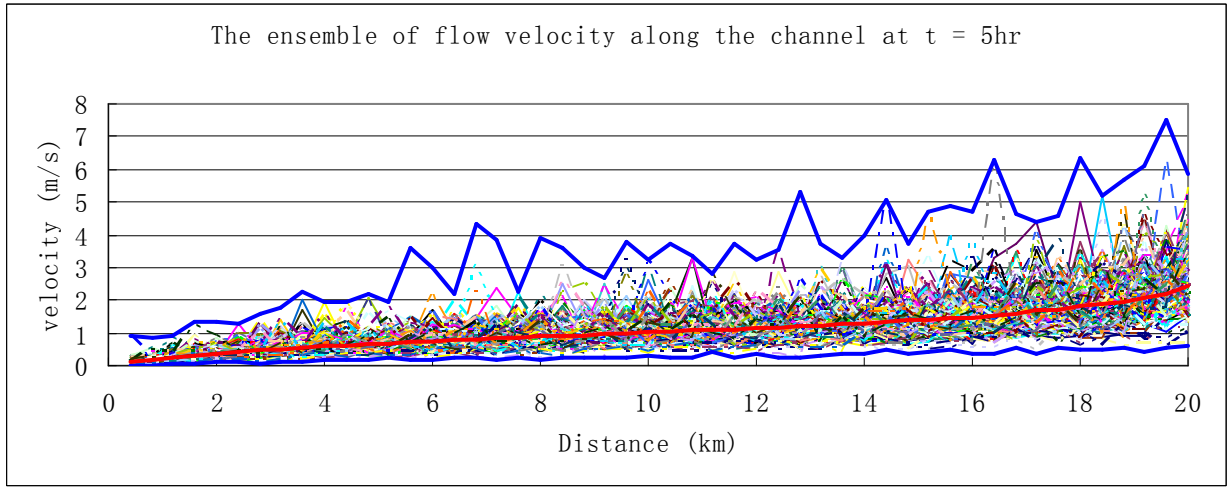
$$Q_I = f(h_I) = \frac{1}{n} A_I R_I^{2/3} S_0^{1/2}$$

where I is the index of downstream cross-section. Since the bed width, Manning's roughness coefficient and bed slope are random, the downstream conditions of Q_I and h_I are uncertain.

The initial condition was computed by assuming steady flow along the channel. The initial flow rate Q at the downstream boundary equals the summation of the initial flow rate at the upstream boundary and the total initial lateral inflow rate along the reach. Since the flow at the downstream boundary is assumed as normal flow, the initial depth h at the downstream boundary is computed based on normal flow equation. Once the initial flow rate and depth at the downstream boundary are computed, the standard step method, a popular method to compute steady flow with a known downstream boundary condition, is applied to establish the initial conditions for Q and h along the channel.

The ensemble of flow velocities along a river reach





Solute transport equation with uncertain parameters:

$$\frac{\partial C}{\partial t} = -U' \frac{\partial C}{\partial x} + D' \frac{\partial^2 C}{\partial x^2} + K'C + S'$$

where U', D', K', S' are uncertain. The values of U' are generated from the ensemble of flow fields.

Modeling the uncertain solute concentration within the framework of uncertain parameters

1. Corresponding to each set of flow parameters, also generate a set of uncertain transport parameters, such as lateral solute concentration of non-point sources, reaction rate, and point source solute, used in the transport equation.

   As such, generate 700 realizations of solute transport along a river channel reach, by means of the solution of the solute transport equation 700 times, each solution corresponding to one set of realized flow and transport parameters.

2. Compute the ensemble average solute concentration along the river reach with four approaches:

   a) Ensemble average of the 700 realizations, simulated by the Monte Carlo method;

   b) Deterministic solution of the transport equation by average flow and transport parameters used in de Saint Venant and solute transport equations;

   c) Ensemble average transport equation with complete 2nd order closure (all seven covariance integral terms accounted for);

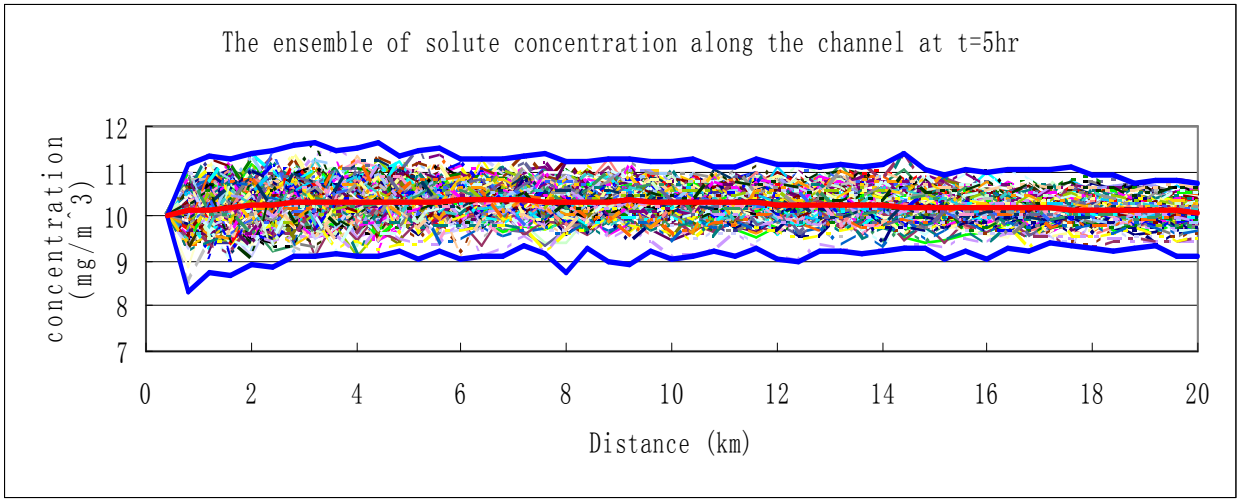
   d) Ensemble average transport equation with 2nd order closure where only the macrodispersion term is accounted for.

For the upstream boundary condition, the solute concentration at the upstream boundary is taken equal to 10 mg/m^3.

As for the downstream boundary condition, the transport equation through a backward finite difference scheme for the downstream node will be consistent with the numerical solution of the transport equation by the central difference scheme at the rest of the spatial grid nodes throughout the whole computing field to render a matrix to be solved.

For the initial condition, the solute concentration along the channel reach is taken equal to 5 mg/m^3.

The ensemble of solute concentration realizations along the channel reach



Ensemble average form of the equation for transport by unsteady river flow under uncertain conditions (exact 2nd order closure):

$$\frac{\partial < C >}{\partial t} = -U'' \frac{\partial < C >}{\partial x} + D'' \frac{\partial^2 < C >}{\partial x^2} + K'' < C > + S'' \qquad (11)$$

$$D'' = < D' > + \int_0^t ds Cov_0 \left[U'(x_t, t); U'(x_{t-s}, t-s) \right]$$

Macro-dispersion coefficient

$$U'' = < U'(x_t, t) > - \int_0^t ds Cov_0 \left[U'(x_t, t); \frac{\partial U'(x_{t-s}, t-s)}{\partial x} \right] + \int_0^t ds Cov_0 \left[K'(x_t, t); U'(x_{t-s}, t-s) \right]$$

1st convection-correction coefficient 2nd convection-correction coefficient

$$K'' = < K'(x_t, t) > - \int_0^t ds Cov_0 \left[U'(x_t, t); \frac{\partial K'(x_{t-s}, t)}{\partial x} \right] + \int_0^t ds Cov_0 \left[K'(x_t, t); K'(x_{t-s}, t-s) \right]$$

1st reaction-correction coefficient 2nd reaction-correction coefficient

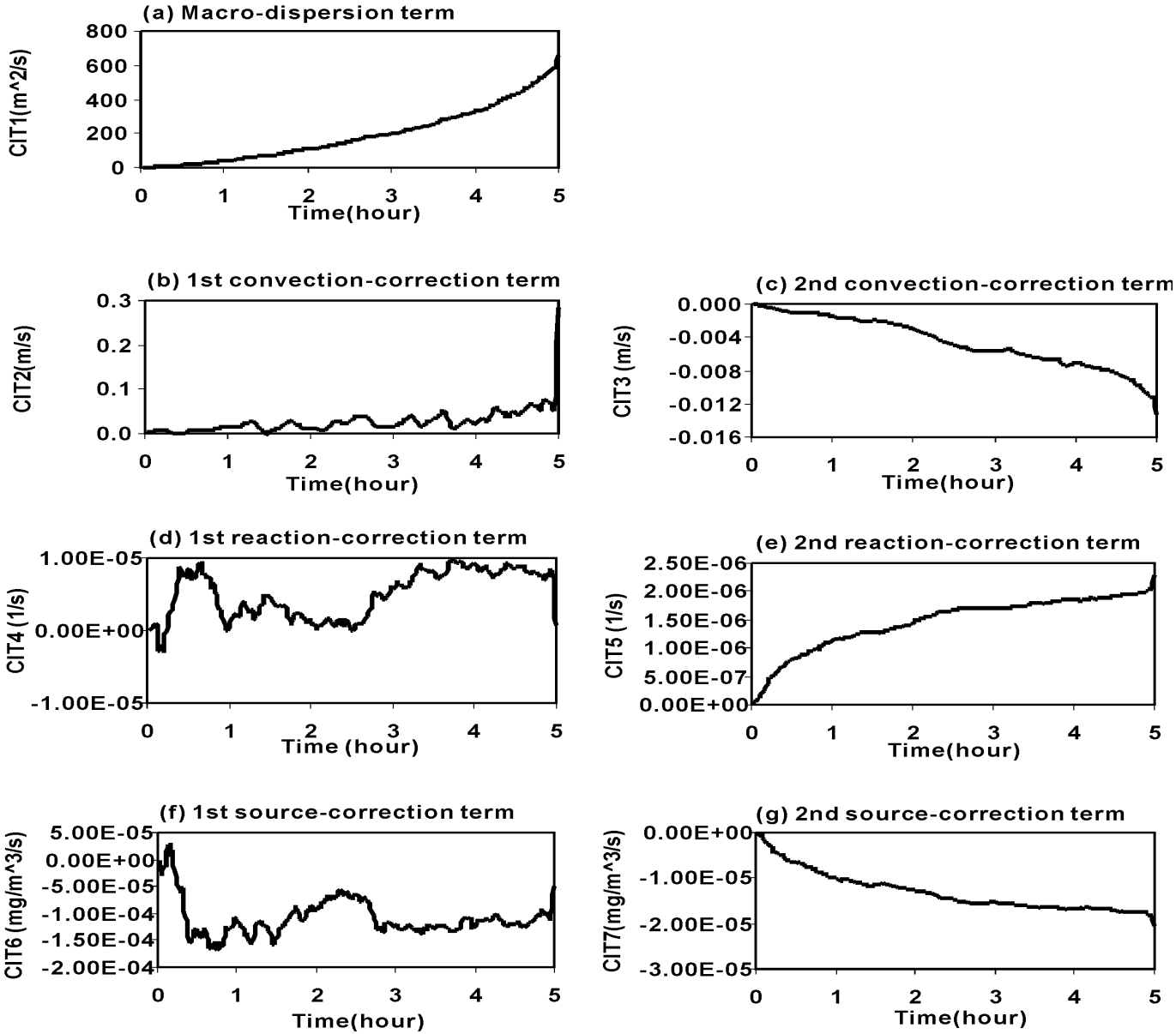
$$S'' = < S'(x_t, t) > - \int_0^t ds Cov_0 \left[U'(x_t, t); \frac{\partial S'(x_{t-s}, t-s)}{\partial x} \right] + \int_0^t ds Cov_0 \left[K'(x_t, t); S'(x_{t-s}, t-s) \right]$$

1st source-correction coefficient 2nd source-correction coefficient

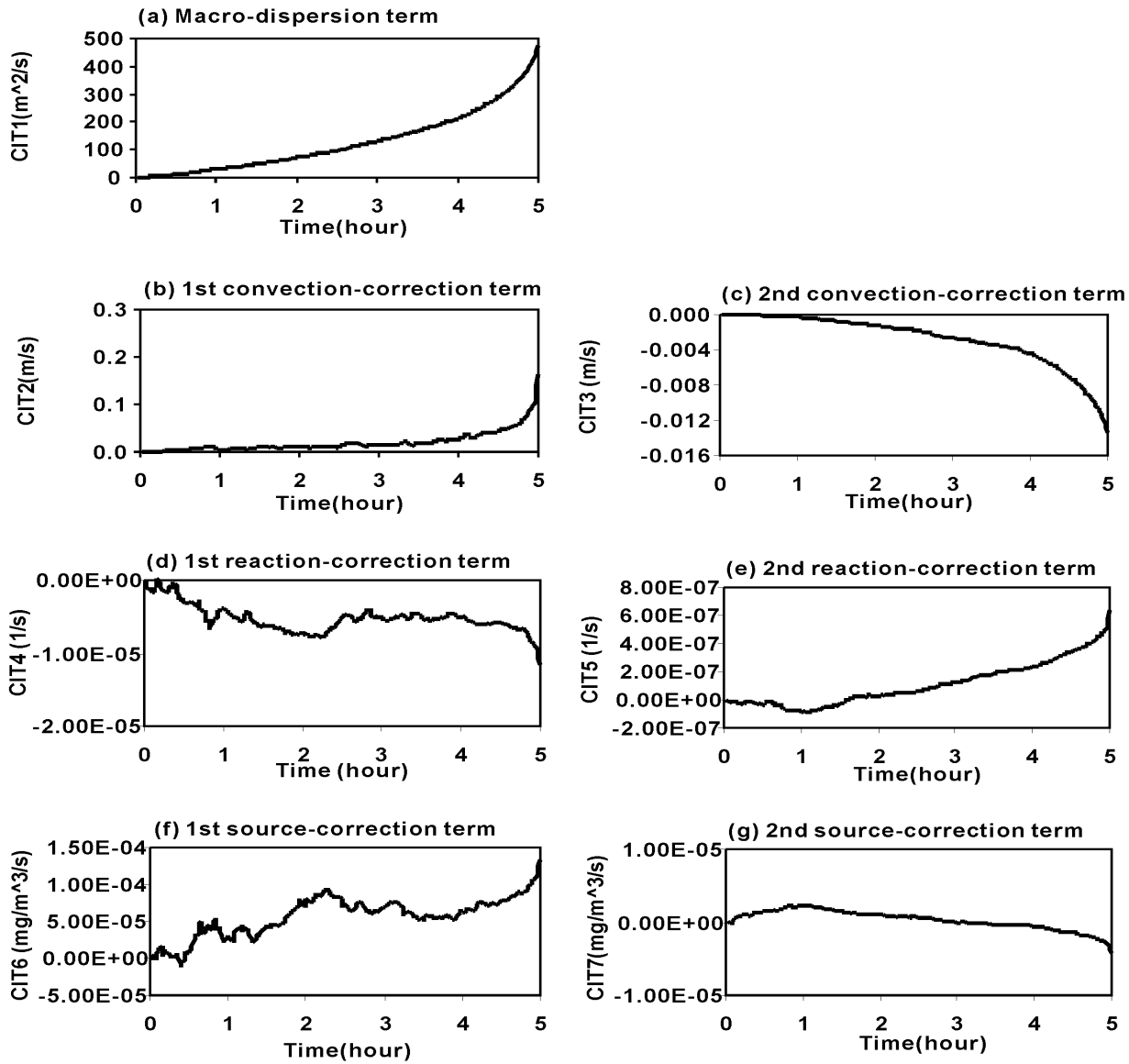
* The **Lagrangian trajectory** of the flow field from the initial time to the time of interest used in the covariance integral terms is expressed as:

$$x_{t-s} = \overleftarrow{\exp}[x, t] x_t = x_t - \int_{t-s}^t d\tau < U'(x, \tau) >$$

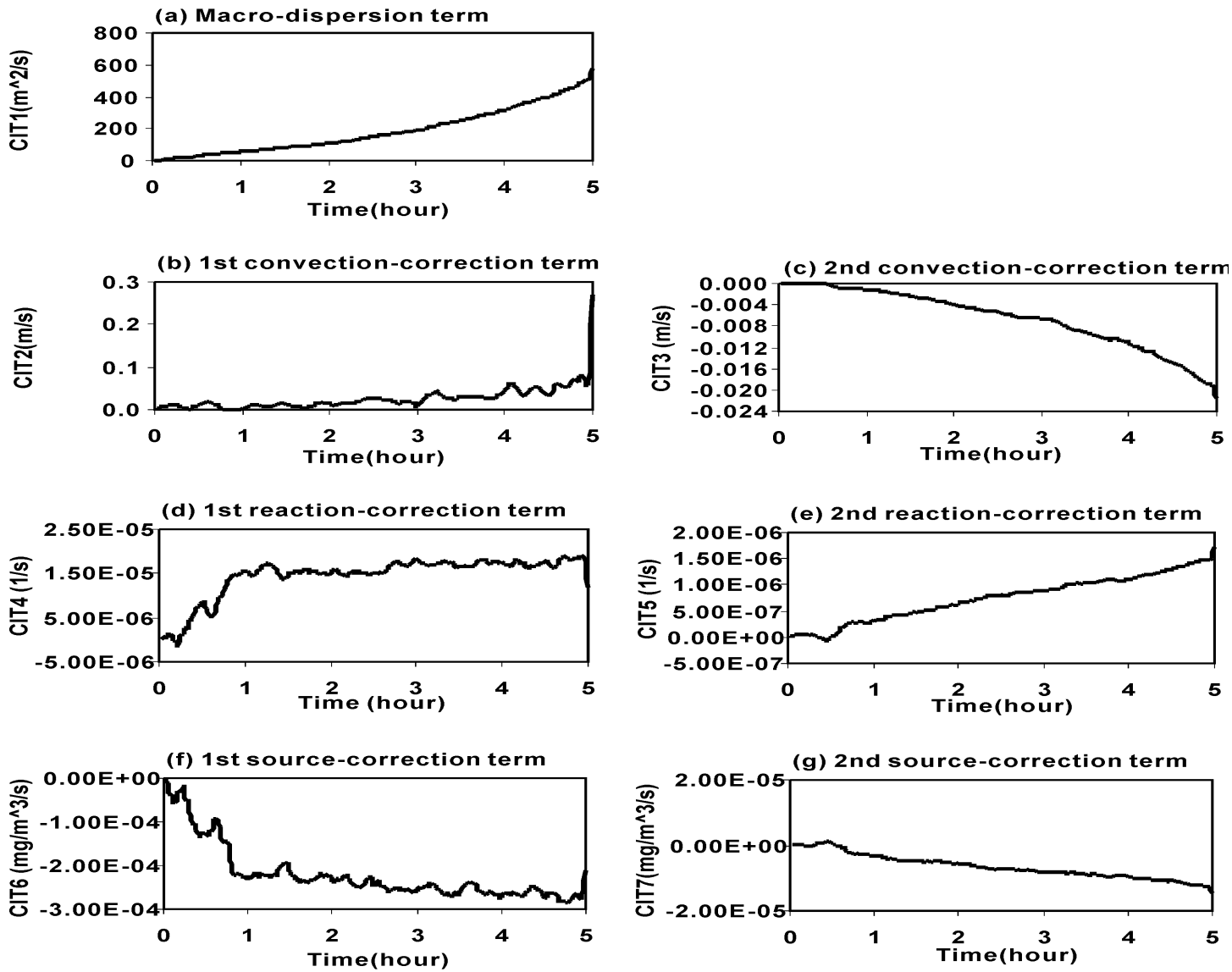
Case 1 - Seven covariance integral terms (CITs) along the mean velocity trajectory at the computational node with x = 20km and t = 5hour



Case 2 - Seven covariance integral terms (CITs) along the mean velocity trajectory at the computational node with x = 20km and t = 5hour



Case 3 - Seven covariance integral terms (CITs) along the mean velocity trajectory at the computational node with x = 20km and t = 5hour



Macrodispersion coefficient for transport by unsteady flow

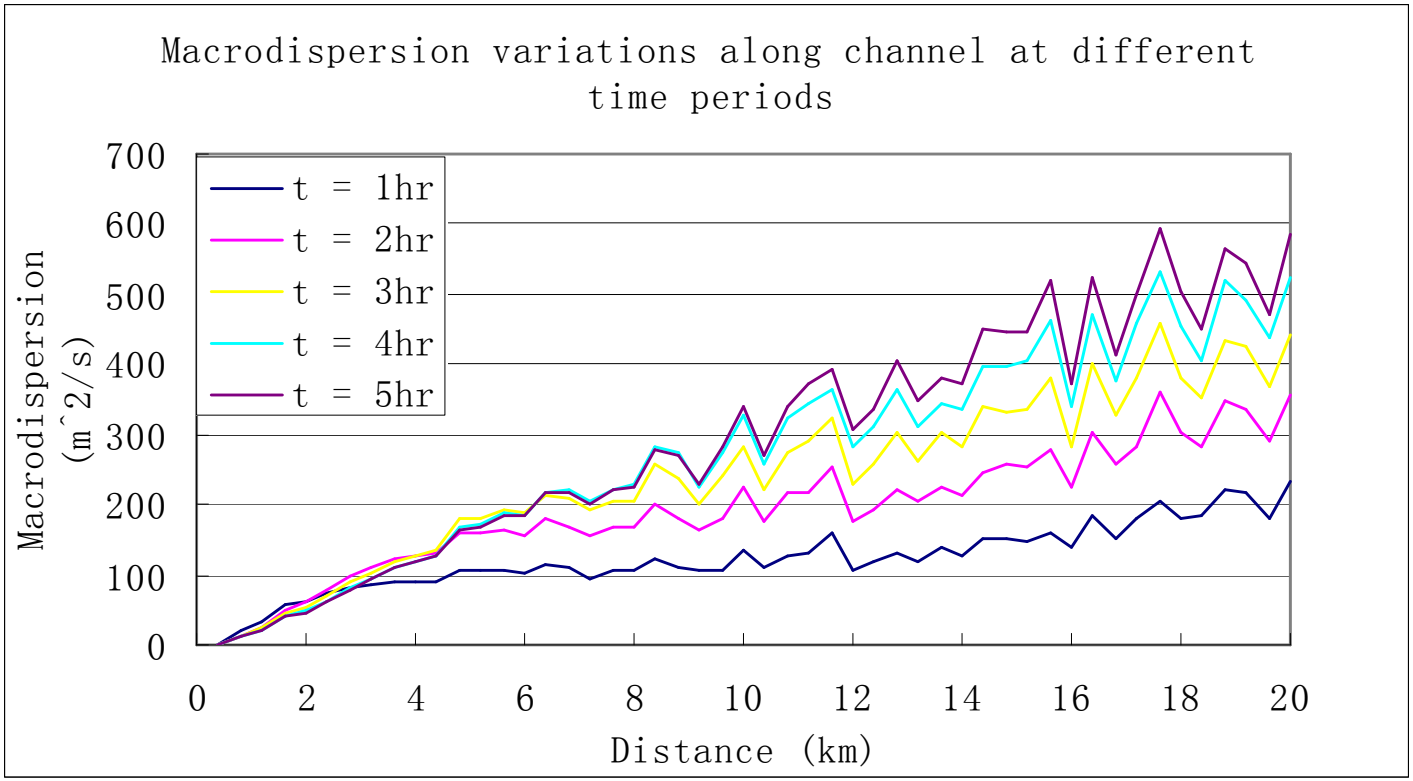
(Kavvas and Karakas, 1996; Kavvas, 2001)

$$\int_0^t ds Cov_0\left[U'\left(x_t, t\right); U'\left(x_{t-s}, t-s\right)\right]$$

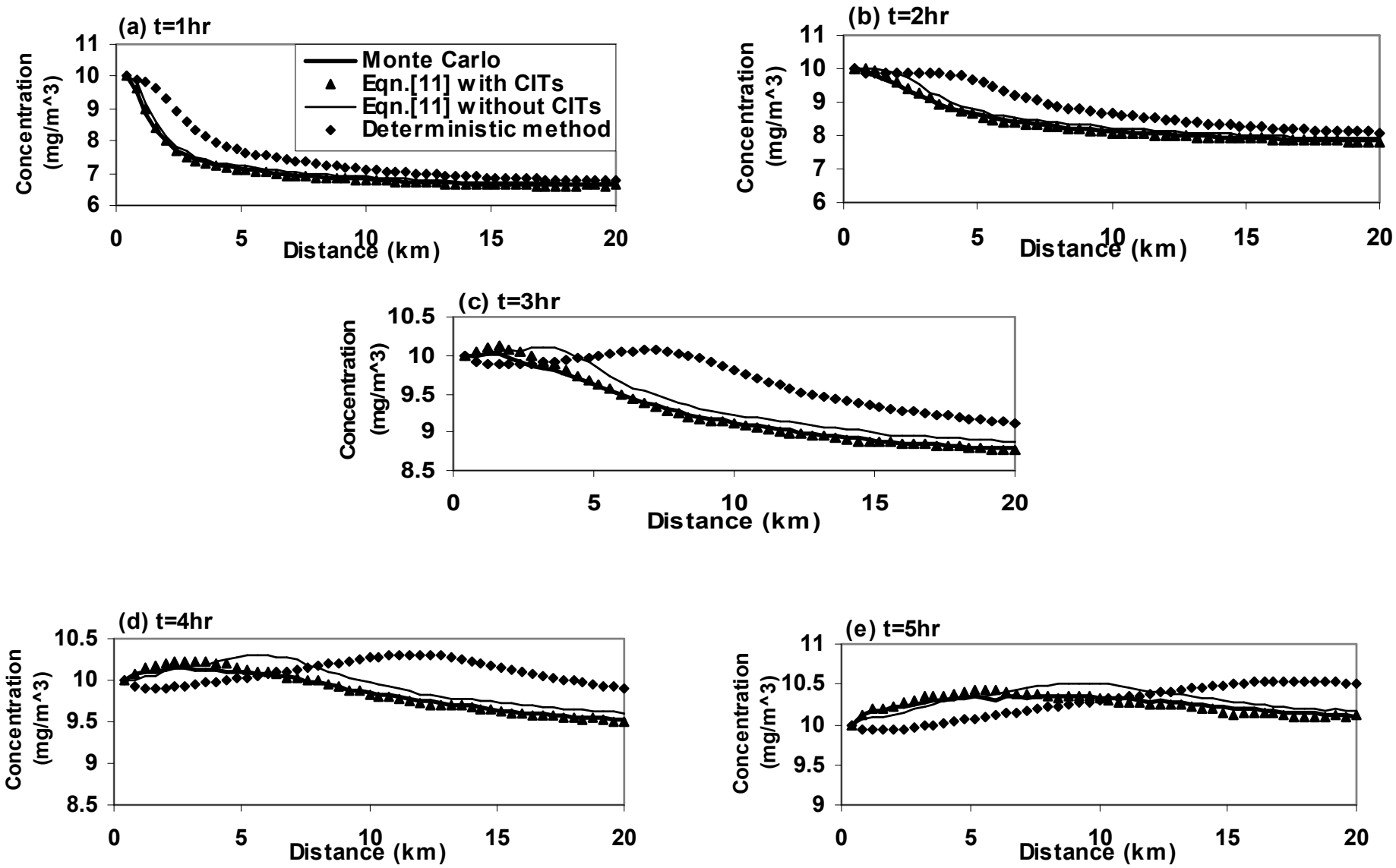
The **Lagrangian trajectory** of the flow field from the initial time to the time of interest used in the covariance integral terms is expressed as:

$$x_{t-s} = \overleftarrow{\exp}\left[x, t\right] x_t = x_t - \int_{t-s}^{t} d\tau < U'\left(x, \tau\right) >$$

Macrodispersion term changes in time and space



Case 3 - Spatial variations of solute concentration for five time periods with four methods:
1. the Monte Carlo method; 2. the ensemble average method with the second order closure;
3. the ensemble average method with the first order closure; 4. the deterministic method.



CONCLUSIONS

1. The solute transport simulation results by the Monte Carlo method are well-replicated by the ensemble average transport equation.

2. Technology is available to determine the macrodispersion coefficient for transport by unsteady river flow. The magnitude of the macrodispersion term is much larger than of those terms that quantify fluctuations in the solute concentration due to other causes (such as the effect of nonuniformity of the flow field on convective motion, the uncertainty in the reaction rate, the uncertainty in the solute sources/sinks).