# Two-Phase Porous Medium Transport Morphological Approach and Optimum Design Applications in Energy Engineering

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**ABSTRACT**

One of the aims for the present work is to depict and outline the possibilities for physically evidencing and explaining optimal design procedures for transport in porous structures which could be used in different engineering fields. Applications range from heat- and mass exchangers and reactors in mechanical engineering design to environmental engineering usage. The latest applications are namely urban air pollution optimal control of pollutant's levels in contaminated areas and design of optimal control point network for the control of constituent dispersion and remediation action design. Using second order turbulent models, equation sets were obtained for turbulent filtration and two-temperature or two-concentration diffusion in non-isotropic porous media and interphase exchange and micro-roughness. The previous works have shown that the flow resistance and heat transfer over highly rough surfaces or in a rough channel or pipe can be properly predicted using the technique of averaging the transport equations over the near surface representative elementary volume (REV). Prescribing the statistical structure of the capillary or globular porous medium morphology gives the basis for transforming the integral-differential transport equations into differential equations with probability density functions governing their coefficients and source terms. Several different closure models for these terms for some uniform, non-uniform, non-isotropic and specifically random non-isotropic highly porous layers were developed. A model of turbulent flow and two-temperature heat transfer in a highly porous medium was evaluated numerically for a layer of regular packed particles. Quite different situations arise when described processes occuring in unregular or random morphology. Latest results obtained with the help of exact closure modeling for canonical morphologies open a new field of possibilities of purposefully searching for optimal design of spacial heterogeneous transport structures. A way to find and govern momentum transport through a capillary nonintersecting medium by altering its morphometrical characteristics is given as validation of the process.

## 1. INTRODUCTION

The averaging of processes in randomly organized heterogeneous media can be performed in different ways. Quintard and Whitaker (1988) and Plumb and Whitaker (1990) have dealt with many questions of determination of transport characteristics in the case of different-scale (two- or three-) nonhomogeneity of the porous medium.

Travkin and Catton (1992a) discussed alternate forms for the mass, momentum and heat transport equations recently presented by various reserchers. The alternate forms of the transport equations are often quite different. The differences among the transport equation forms advocated by the numerous authors displays the fact that research on basics of governing equations of transport processes in porous media is still an evolving field of study. Derivation of the equations of turbulent flow and diffusion for a highly porous medium during the filtration mode is based on the theory of averaging by certain REV )S of the turbulent transfer equation in the liquid phase and transfer equations in the solid phase of the heterogeneous medium (see, for example, Whitaker 1967, 1986a, for laminar regime developments and for turbulent filtration by Scherban et al. 1986, Primak et al. 1986, and Travkin and Catton 1992a, 1993a). The whole sets of 3-D and 2-D boundary equations of developed turbulent transfer in a stationary porous medium with penetration resulted in papers by Scherban et al. (1986) and by Travkin and Catton (1992a,b and 1993a ).

A very important, unresolved question in heterogeneous modeling concerns the conformity of one- and two-temperature or two-concentration models. The theory of homogenization has been rigorously developed currently only for the classical equations of mathematical physics with constant coefficients. To solve this effective coefficient problem, which seems misleadingly simple from a physical point of view, the entire series of similar boundary value problems should be solved . It means that if computer and framework capabilities allow one to model two-concentration process that occurs then the less incorrectness will be involved in the results.

## 2. SIMPLIFIED 2D TURBULENT FORCED TRANSPORT GOVERNING EQUATIONS IN HIGH PERMEABILITY MEDIUM

Turbulent transport equations for a single phase fluid in a highly porous random media have more integral and differential terms than in the convenient homogenized or classical continuum mech\anics equations. Various descriptions of the porous media structural morphology determine the importance of these terms and the range of application of closure schemes. For example, a simplified two-dimensional transverse equation of momentum in a randomly homogeneous porous medium within a boundary area between two layers under steady-state conditions and other simplifications, with no flow penetration through interface surface $MS_w$, for a horizontally homogeneous stream, has the form (Travkin and Catton 1992b,Travkin et al. 1993b)

$$\frac{\partial}{\partial z}\left(\langle m\rangle\left(\tilde{K}_m + \nu\right)\frac{\partial \tilde{\bar{u}}}{\partial z}\right) + \frac{\partial}{\partial z}\left(\langle \hat{K}_m \frac{\partial \hat{\bar{u}}}{\partial z}\rangle_f\right) + \frac{\partial}{\partial z}\left(\langle -\hat{\bar{u}}\hat{\bar{w}}\rangle_f\right) =$$

$$-\frac{1}{\Delta\Omega}\int_{\partial S_{wT}}\left(K_m + \nu\right)\frac{\partial \bar{u}}{\partial x_i}\cdot d\vec{s} + \frac{1}{\rho_f\Delta\Omega}\int_{\partial S_w}\bar{p}\, d\vec{s} + \frac{1}{\rho_f}\nabla\langle\bar{p}\rangle_f =$$

$$u^2_{*rk}S_w(z) + \frac{1}{\rho_f\Delta\Omega}\int_{\partial S_w}\bar{p}\, d\vec{s} + \frac{1}{\rho_f}\nabla\langle\bar{p}\rangle_f\,, \tag{1}$$

where "~" means the value averaged over the REV liquid phase volume, and $<>_f$ means averaging over the REV, "^" means fluctuations of mean turbulent variables in the fluid domain, and where $u^2_{*rk}$ is the dynamic velocity at the upper boundary of the microroughness layer in a pore scale of thickness $h_r$, averaged over internal REV surface $MS_w$.

The generalized longitudinal 1D mass transport equation in fluid phase, including description of potential morpho-fluctuation influences, for the medium morphology with the only 1D fluctuations is written as follows,

$$\frac{\partial}{\partial x}\left[<m>(\tilde{K}_c + D_f)\frac{\partial \tilde{C}(x)}{\partial x}\right] + \frac{\partial}{\partial x}\left[<m>\{\hat{K}_c\frac{\partial \hat{C}(x)}{\partial x}\}_f\right] +$$

$$\frac{\partial}{\partial x}\left[<m>\{-\hat{\tilde{u}}\hat{C}\}_f\right] + \frac{\partial}{\partial x}\left[\frac{(\tilde{K}_c + D)}{\Delta\Omega}\int_{\partial S_w}\hat{C}\, d\vec{s}\right] +$$

$$\frac{1}{\Delta\Omega}\int_{\partial S_w}(K_c + D_f)\frac{\partial\bar{C}}{\partial x_i}\cdot d\vec{s} + <m>\tilde{S}_c = <m>\tilde{u}\frac{\partial\tilde{C}}{\partial x}\,, \tag{2}$$

where C is concentration, $K_c$ and $K_m$ in (1) are turbulent eddy diffusivity and viscosity.

There are 4 terms in each of the equations that need to be modeled in some way. A few closure equations for the first and the second terms on the right hand side in (1) and integral term in (2) were introduced and numerically evaluated by Travkin and Catton (1992a,b,c) and Gratton et al. (1993) for typical regular or nonstructured porous media. Closure models allow one to find connections between experimental correlations for bulk processes and the present simulation representation and to incorporate them into numerical procedures. Modeling of the third term on the left hand side of the above equation presents a problem whose features remind one of the main disturbance theory problem. The substantial difference between turbulence covariance closure of the fluctuations and the present situation consists of knowledge that the covariances of "morpho-fluctuations" are determined by the morphology of the medium in the vicinity of the fluctuation occurrence, whereas the covariances of the values can be determined by proceeding from the experimental morphometric data for the porous medium. At the present time, not many experimental studies of sufficient accuracy have been done to show the difference between random and regular (periodic) structure of the bed's granules.

An admitted or assigned statistical structure of the capillary or globular porous medium morphology gives the basis for transforming integral-differential transport equations into differential equations with probability density functions governing the stochastic coefficients and source terms. There were introduced and developed morphological models that simulate turbulent transport of momentum, mass and heat in an environment that can be represented as different structure networks. For classical cases of parallel tube bundles with assigned nonregular or stochastic distributions of morphology characteristics such as tube diameter and porosity, analytical expressions can be obtained for bulk characteristics, like overall drag resistance coefficient $c_d$.

Terms with components of the Reynolds stress tensor in averaged equations, and similar terms for heat or mass transfer, are complemented by covariant functions of fluctuations of quantities caused by the porous medium morphology

$$< \hat{\overline{U}}_j \, \hat{\overline{U}}_i >_f \quad , < \hat{\overline{U}}_i \, \hat{\overline{C}} >_f , < \hat{K}_c \, \frac{\partial \hat{\overline{C}}}{\partial x_i} >_f \quad , < \hat{K}_m \, \frac{\partial \hat{\overline{U}}}{\partial x_i} >_f ,$$

can be considered as the control additives in the transport equations. A known or assigned morphological characteristics actually allow one to perform process optimization. Herewith, all of the functions might be either an analytical expressions determined with the aid of approximate theoretical evaluation or numerically obtained or experimental dependencies.

## 3. APPLICATIONS IN MECHANICAL AND ENVIRONMENTAL ENGINEERING

The next presented applications have the common similarities in their mathematical implementation which could naturally substantiate the outline for a specific class of optimal design models.

### 3.1. Heterogeneous Heat Transfer Surfaces

Turbulent transport phenomena can be considered in a sufficiently large channel (pore) with account of roughness on the wall using the same averaging approach. This method allows the treatment of complex morphology structures, even combinations of different structure types (e.g. a channel with rough walls and porous inlay). Averaging the transport equations over the REV by the method developed in the works by Shcherban et al. (1986), Primak et al. (1986), and Primak and Travkin (1989) allows investigation of virtually an unlimited variety of morphology structures in a channel. The basics for using the technique were developed for atmospheric urban boundary layer

(Shcherban et al. 1986, and Primak et al. 1986), rough wall channels with turbulent transport of matter and for highly porous media studied recently by Travkin and Catton (1994a).

The horizontal dimensions of the REV are far greater than the characteristic dimensions of the roughness elements in longitudinal direction and infinite in transverse direction. In the case of regularly arranged roughness elements the longitudinal dimension of one REV is typically one pitch of the roughness elements. Independent treatment of turbulent energy transport in the fluid phase and energy transport in the solid phase, connected through the specific surface (the solid-fluid interphase in the REV) allows a more accurate modeling of the heat transfer mechanisms between the rough surface and the fluid phase. In the transport models was used one additional term as a control term for regular spatial 2D and 3D rough layer morphologies.

### 3.2 Regular Heat and Mass Exchange Spacial Structures

The turbulent transport statement set was also constructed for the case of turbulent flow in a highly porous layer combined with a two energy equation model. The transfer equations for each of the phases are used with some simplification, determined by the turbulence order and medium regularness (Travkin and Catton 1992a). Models for transport coefficients were derived with real consideration of the medium morphology that put forward an introduction of a different averaging technique. The closure model is simple and presents a clear physical problem statement as well as incorporating three additional terms. It was shown (Travkin and Catton 1992a,b) that most experimental correlations can be related to the present work. In considering a porous medium canonically formed from tubes and slits, we reviewed some existing theoretical derivations and unify the various points of view and conclusions.

More precise description of the layer morphology in the case of cubic geometry illustrates the effects of local structure variation upon the models. It was shown that transport equations are sensitive to the types of morphology assumed and the descriptive ability of the transport coefficients used which were actually the controls in the equations. Some models and transfer equations were developed in Komkov et al. (1987) for abatement of gas power station effluents in multisection gascleaning reactors with liquid phase. Flow, heat and mass transfer simulation was made for a hollow section and packed bed section of reactor with concurrent and countercurrent flow of gaseous and liquid phases. The transfer equations were obtained on the basis of formalism described above in simplified form for two- and three-phase media turbulent transfer: the disperse liquid phase, the liquid phase in porous medium and the multicomponent vapor-and-gas mixture of smoke gases with passive and active packing.

### 3.3 Urban Rough Layer Morphological Air Pollution Modeling

One more area of application was explored earlier. The problems of atmospheric diffusion and heat pollution in large urban settlements be formulated with an allowance for the interaction of the atmospheric boundary layer (ABL) with an underlying surface consisting of urban roughness layer (URL) obstacles. In an urban area, the main features of an analysis are the nonhomogeneity of the distribution of pollution sources in space and the problem of description or parameterization of the underlying surface roughness.

A morphometric technique technique for obtaining a mathematical description of surface with a randomly nonhomogeneous roughness layer has been elaborated on by Scherban et al. (1986). The technique is different from the few known methods (Khusu et al. 1975, Das 1984) and is based upon the analysis of morphometric characteristics obtained in the so-called elementary statistical volumes (ESV), into which the roughness layer is divided.

Among the morphometric characteristics of the distribution densities to be calculated and evaluated were the distribution densities of surface and volume porosities, of distances between the obstacles and their granular composition, of heights and specific surface of obstacles.

The results of these modelings have been applied to the problem of pollutant transfer in URL in cities and industrial centers (Scherban et al. 1986, Primak et al. 1986). These models offered not general, but strictly experimental allowance for the morphological characteristics of the randomly nonhomogeneous roughness layer of urban housing systems and phytocenosis and make it possible to assess their effect on the characteristics (controls) of the turbulent boundary layer and diffusion of harmful impurities in the URL layer.

### 3.4 Groundwater and Soil Contamination Modeling

The morphologies of various geological materials involve high porosity and high permeability solid media. Some of the media with well examined lithologies include volcanic rock formations with bulk permeabilities on the order of thousands of Darcies and young dolomite or limestone reservoirs with porosities as large as 60%. The inclusion of soil sciences allows the consideration of solidified surface magmas and tropical soils with porosities exceeding 60% and of regions deforested by fire with silts consisting of activated charcoals providing void fractions above 80%. Equations for the transport processes occurring in such randomly anisotropic soil media were developed using a hierarchial modelling methodology which incorporates a successive-scale approach ultimately rendering the governing equations set for the macrovariables (Travkin et al. 1994c).

## 4. VARIETY OF OPTIMAL CONTROL PROBLEMS WITH DISTRIBUTED PARAMETERS AND CONTROLS DETERMINED BY POROUS MEDIUM MORPHOLOGY

The optimal control problems involving the equations like (1), (2) having the control terms structured as following

$$
\begin{gathered}
\nabla\,(<m>\{f_1(\vec{x})\,\nabla f_2(\vec{x})\}_f)\,,\ \nabla\,(<m>\{f_3(\vec{x})\ f_2(\vec{x})\}_f)\,, \\
\nabla\,(\varphi_1 \int\limits_{\partial S_w} f_2(\vec{x})\,\vec{ds})\,,\ \int\limits_{\partial S_w} (\varphi_2(\vec{x})\,\nabla\,(f_4(\vec{x}\,,f_2(\vec{x}))))\,\vec{ds}\,,
\end{gathered}
\tag{3}
$$

with controls $f_1$, $f_2$, $f_3$, $f_4$. These statements of control problem are barely seen in contemporary literature regarding the optimal control distributed parameter systems (see, for example, Fattorini 1985,1994). The existance of optimal controls for equations much simpler than presented in section 2 were proven only in the latest studies. Thus for linear heat- and mass diffusion problems with the impulse control functions of magnitude or spatial locations of impulses Aniţa (1994) got the formulation of maximum principles for both optimal problems. Ahmed and Xiang (1994) proved the existence of optimal controls for clear nonlinear evolution equations on a Banach spaces. Meanwhile, the control term in the equations was represented as an additive-multiplicative term B(t)u(t).

Reduction of "heterogeneous" terms in the corresponding momentum equation (1) yields, by the overall representation of diffusive and "diffusion-like" terms

$$
K_{m,eff}\,\frac{\partial \tilde{u}}{\partial z} = \left( \langle m \rangle\,(\tilde{K}_m + \nu)\,\frac{\partial \tilde{u}}{\partial z} + \langle \hat{K}_m\,\frac{\partial \hat{u}}{\partial z} \rangle_f + \langle -\hat{u}\,\hat{w} \rangle_f \right). \tag{4}
$$

Here the variables of velocity and changeble viscosity coefficient are taken in form suitable for both laminar and turbulent flow regimes.

For problems with a constant bulk viscosity coefficient ($K_m$ = constant) the second term in this relation vanishes and the whole problem essentially assumes the role of evaluating the influence on the momentum due to dispersion by irregularities of the soil medium. Diffusion-dispersion effects realized through the second derivative terms and relaxation terms in the fluid phase mass transport equation can be expressed,

$$
\begin{gathered}
K_{c,eff}\,\frac{\partial \tilde{C}}{\partial x} = [<m>(\tilde{K}_c + D_f)\,\frac{\partial \tilde{C}}{\partial x} + <m>\{\hat{K}_c\,\frac{\partial \hat{C}}{\partial x}\}_f - \\
<m>\{\hat{w}\,\hat{C}\}_f + \frac{(\tilde{K}_c + D_f)}{\Delta\,\Omega} \int\limits_{\partial S_w} \hat{C}\,\vec{d}s]\,,
\end{gathered}
\tag{5}
$$

where the first and last terms resemble the effective thermal conductivity coefficient for each phase, using constant coefficients, in the work by Nozad et al. (1985). By pretending the control terms to be as an additives to the bulk transport coefficients represents the another variation in optimal control mathematical statement.

## 5. EXAMPLES OF OPTIMAL CONTROL SIMULATIONS IN CANONICAL MORPHOLOGIES OF POROUS MEDIUM

A statement for intense heat and momentum transport was simulated and evaluated by Travkin and Catton (1992b) and Gratton et al. (1993). These works numerically investigated the effects of local morphology and flow characteristics upon the bulk medium and flow properties. Transport processes in unconsolidated, non-structured single-size spherical packings, regular single-size spherical packings, straight, equivalent capillary tube morphologies, and a bi-porous medium structure, consisting of capillaries with internal obstacles, were studied numerically. The prescribed local morphological structures were shown to clearly manifest themselves in the order of magnitude of the predictions given for both local and bulk flow parameters using extensions of experimental data for single-porous medium structural elements (e.g. the coefficient for a single bead, or single straight pore) to subsequently calculate bulk transport coefficients.

The morphology of straight capillary medium possess the following features:

1) the space distribution of pores is stationary in a broad sense in the lateral direction and accordingly, the same feature for velocity deviations should be admitted;

2) the second morpho-diffusive term on the left hand side [Eq.(1)], if there is not an artificially assigned momentum transport or exchange in the lateral direction, no longer requires retention;

3) to simplify analytical derivations, the assumed independence of momentum transport from lateral coordinate far from the interface surface contributes to the first left-hand side term [Eq.(1)] vanishing also.

To assert the differentiability of random functions of the morpho-diffusive term in the momentum equation, specific conditions should be assumed for this morphology. Consideration of those features which happen to exist in the equation due to this specific type of porous medium reduces the equation governing the flow of fluid to the two term expression

$$-\nabla \tilde{p} = c_d \left( \frac{S_w}{<m>} \right) \frac{\rho_f \tilde{u}^2}{2} . \qquad (6)$$

For purely qualitative analysis, the adoption of non-permeable interphase boundaries precludes mass transfer at the pore walls and consequently allows omission of the integral terms. The equation then acquires the form

$$\frac{\partial}{\partial x}\left[ (\tilde{\mathrm{K}}_c + D_f) \frac{\partial \tilde{C}(x)}{\partial x} \right] + \frac{\partial}{\partial x}\left[ \{ \hat{\mathrm{K}}_c \frac{\partial \hat{C}(x)}{\partial x} \}_f \right] +$$

$$\frac{\partial}{\partial x}\left[ \{ -\hat{u}\hat{C} \}_f \right] + \tilde{S}_c = \tilde{u} \frac{\partial \tilde{C}}{\partial x} , \qquad (7)$$

where at least averaged dispersivity coefficient can be directly calculated alongside with the two morpho-terms (the second and the third in the left hand side of (7).

**CONCLUSION**

Common occurrence in porous media modelling is the inverse problem, requiring the calculation of many coefficients.
The exact closure procedures is derived from a capillary type morphology description at the pore scale. The elementary macrovolume morphologies considered are systems of straight-equivalent channels with anisotropic features and random morphology fluctuations.

Further simplifications of the governing equations and considered morphology allow preliminary results showing that the method has advantages over simple, deterministic Darcy law based treatments with constant coefficients. The parameter $S_w$ exerts great influence upon the bulk flowfield, through the drag coefficient, by the mechanism of fluid-friction. The simple preliminary treatments are incapable of accounting for random variations of the solid medium and result in large magnitude error if coefficients are not chosen to correspond to the bulk flow regime and morphology of the real physical situation being modelled.

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