ON THE RELATIONSHIP BETWEEN MULTIPLE POROSITY MODELS AND CONTINUOUS TIME RANDOM WALK

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Summary. We derive a multiple porosity model based on the continuous time random walk model (CTRW). In particular, we show how the parameters of the multiple porosity models relate to the transition probability function which is at the heart of the CTRW formulation. A simple example is included to illustrate the results.

1 INTRODUCTION

Models for particle transport associated with fluid flow in porous media are essential for a wide range of applications spanning exploitation of groundwater resources to paper production and fuel cells. While many of the challenges in these applications relate to the simultaneous flow of multiple fluids through the pore space, even transport of a passive component flowing with a single fluid is not properly understood on scales above that at which the porous structure can be resolved (see e.g. the special issue [1]).

Numerous experiments indicate that the solutions to the Advection-Dispersion Equation (ADE) and its modifications do not capture the full complexity of transport (see e.g. [2] and references therein). The last decade, the Continuous Time Random Walk (CTRW) model has been advocated as a general framework to address transport in porous media [2]. This is supported by the equivalence to the generalized master equation (GME) [3], showing that the solutions of CTRW must include the solution of all other deterministic transport models either through equivalence or as a subset.

However, in practical applications, multiple porosity models remain much more wide-spread, due to their simple implementation in existing code packages, as well as their simple intuitive interpretation [4, 5].

In this paper, we show an explicit relationship between multiple porosity models and CTRW. This relationship goes beyond the usual analysis, which shows how CTRW converges to certain fractional differential equations in appropriate limits, by defining a multiple porosity model which is identified as identical to CTRW under a certain discretization in its Lagrangian formulation. This is achieved through considering generalized multiple porosity models with potentially infinitely many continua.

Thus, we formulate a duality where CTRW is seen as a spatial discretization of transport, while retaining the exact structure of the subscale velocity distribution. In contrast, multiple

porosity models with a finite number of continua can be considered as spatially continuous models with a discrete approximation to the velocity distribution.

We structure the presentation as follows. In the next section, we give the generalization of multiple porosity models we exploit in this paper. In section 3, we give a brief reminder of the main formulations of CTRW. Finally, in Section 4, we show the explicit relationship between CTRW and multiple porosity models.

2 MULTIPLE POROSITY MODELS

Multiple continua models are the intuitive generalization of single continua models. The idea was first presented by Barenblatt [6], and has since been widely used, not only for particle transport but also for multi-phase flow and thermal transport.

Most commonly, multiple porosity models are applied to only two continua, and these are then identified as e.g. the fracture continua and the matrix continua. The equation for mass transport in the fracture continua (identified by subscript 1) can then be written as

$$\partial_t m_1 + \nabla \cdot (\boldsymbol{u}_1 \, c_1 - \boldsymbol{D}_1 \nabla c_1) = \kappa \, (c_2 - c_1), \tag{1}$$

with the equivalent transport equation for the matrix continua (identified by subscript 2)

$$\partial_t m_2 + \nabla \cdot (\boldsymbol{u}_2 \, c_2 - \boldsymbol{D}_2 \nabla c_2) = \kappa \, (c_1 - c_2). \tag{2}$$

In equations (1-2), we may relate masses and concentrations by the porosity ϕ and the fraction of the porosity which is associated with each continua φ_i, thus using ρ to denote density, $m_i = \rho \phi \varphi_i c_i$. The fluxes $\boldsymbol{u}_i$ are usually determined from Darcy's law, while the dispersion tensors $\boldsymbol{D}_i$ and interaction coefficient κ are (possibly flux dependent) properties of the medium. We take these parameters as known herein.

The natural generalization of the dual porosity models is the n-porosity model employed by Gwo for contaminant transport [5] and by Pruess for thermal transport [4]. This model can be concisely written as

$$\partial_t m_i + \nabla \cdot (\boldsymbol{u}_i \, c_i - \boldsymbol{D}_i \nabla c_i) = \sum_{j=1}^{n} \kappa_{i,j} \, c_j, \qquad \text{for all} \quad i = 1..n. \tag{3}$$

The parameters $\kappa_{i,j}$ must be positive (when $i \neq j$) for dispersive processes, with $\sum_j \kappa_{i,j} = 0$. Further, we mass conservation implies $\sum_i \kappa_{i,j} = 0$. By definition, we also have the constraint that $\sum_i \varphi_i = 1$.

Herein, we will further generalize Equation (3) by considering not only a finite number of continua, but indeed infinite families of continua. On one hand, this is simply a formal generalization, but it may also be given physical interpretations as we will see below. When we treat the index as a continuous variable, we will denote it by ω, which is assumed to be in the space Ω. Our independent variables are then functions of both physical and parameter spaces, in addition to time, e.g. $m = m(\boldsymbol{x}, \omega, t)$, where $(\boldsymbol{x}, \omega, t) \in \mathbb{R}^d \times \Omega \times \mathbb{R}^+$. The continuous generalization of Equation (3) is then stated as

$$\partial_t m + \nabla_x \cdot (\boldsymbol{u} \, c - \boldsymbol{D} \nabla_x c) = \int_\Omega \kappa(\omega, \omega') c(\omega') \, d\omega'. \tag{4}$$

The subscript on the differential operators emphasizes that the differential is with respect to the spatial coordinate, as opposed to the parameter space coordinate ω.

The generalized multiple porosity model can also be written such that it accommodate non-

passive particles by replacing the integral transform on the right hand side by a non-linear operator, which we write as:

$$\partial_t m + \nabla_x \cdot (\boldsymbol{u}\, c - \boldsymbol{D}\nabla_x c) = N\big(m|_{\boldsymbol{x},t}\big). \tag{5}$$

3 CONTINUOUS TIME RANDOM WALK

The Continuous Time Random Walk (CTRW) models represent a distinct departure from the modeling philosophy of Section 2. Instead of looking at the deterministic movement of a concentration of particles in a continuum, CTRW considers the transition probabilities for particles between discrete points.

The usual CTRW derivation lets the probability density R of a particle arriving at some point in time be related to the history of the problem [7]:

$$R(\boldsymbol{x},t) = \sum_i \int_0^t \psi_{CTRW}(\boldsymbol{x}_i', t') R(\boldsymbol{x} - \boldsymbol{x}_i', t - t')\, dt' \,. \tag{6}$$

Here we use a summation over space to emphasize that the spatial points are discrete and countable, and the transition probability is given by ψ_{CTRW}. From this equation, the probability density P of a particle being at a point is deduced from the probability that it has not transitioned to a different point,

$$P(\boldsymbol{x},t) = \int_0^t \Psi(t') R(\boldsymbol{x}, t - t')\, dt', \tag{7}$$

where the probability of not transitioning is defined as

$$\Psi(t) = 1 - \int_0^t \sum_i \psi_{CTRW}(\boldsymbol{x}_i', t')\, dt', \tag{8}$$

Continuous time models thus shift the emphasis away from the traditional view of advection and dispersion on a continuum scale, towards a concept of a spectrum of transition times. These are useful concepts and ideas, and they motivate our desire to incorporate this approach within multiple porosity models.

4 MULTIPLE POROSITY AND CTRW

We have seen in sections 2 and 3 that while both multiple porosity (MP) models and continuous time random walk aim at describing transport phenomena, they are parameterized by different functions. Indeed, the main parameters of concern to us in the MP model are the flux distributions $\boldsymbol{u}$; the distribution of continua (porosity) φ_i; and the kernel of the continua exchange term κ. In contrast, the important parameter of the CTRW model is the transition probability function ψ. Recalling that our aim is to be able to reproduce the results of CTRW within a MP model, we will in this section show how to chose the parameters of the multiple porosity model given a transition probability function ψ_{CTRW}.

Our approach will be to manipulate the MP model, by change of variables, rewriting the equation in a Lagrangian framework, and finally introducing a low-order quadrature. This will lead to equations equivalent to Equations (6), and we can thus identify the relationship

between the parameters of the two models. Since Equation (6) is discrete in space, we will use a form of the MP porosity model where the parameter space has both continuous and discrete components.

As a preliminary note, we point out that the non-linear MP model is related to the Boltzmann equation, by identifying $\Omega = \mathbb{R}^d$, and interpreting it as the (discrete) flux space, e.g. $\omega = \boldsymbol{u}_i$. We then obtain from a dispersion free Equation (5)

$$\partial_t m_i + \nabla_x \cdot (\boldsymbol{u}_i\, c) = N_i\big(m|_{\boldsymbol{x},t}\big). \qquad (9)$$

Up to the scaling between flux and velocity, Equation (9) is a discrete Boltzmann equation with no body forces. A common approximation to the collision term of the Boltzmann equation is the Bhatnagar-Gross-Krook (BGK) collision operator [8], which takes the form

$$N_{i,BGK}\big(m|_{\boldsymbol{x},t}\big) = \frac{\langle m \rangle\, f_{i,eq} - m_i}{\tau}. \qquad (10)$$

Here angled brackets implies integration and summation over the parameter space Ω;

$$\langle m \rangle = \langle m \rangle(\boldsymbol{x}, t) = \int_\Omega m(\boldsymbol{x}, \omega, t)\, d\omega = \sum_i \int_{\Omega_c} m_i(\boldsymbol{x}, \omega_c, t)\, d\omega$$

Here, Ω_c refers to the continuous part of Ω. Further, the equilibrium distribution refers to the distribution in Ω, such that $f_{eq} = f(\omega; \boldsymbol{x}, t)$. Note that for dispersive processes, Equation (10) implies that $f_{eq} = \varphi$, since $m = \rho\phi\varphi c$. The characteristic time-scale of relaxation is given by τ, and we will include this time-scale in the parameter space, thus $\Omega = \mathbb{P} \times \mathbb{R}^+$, and $\omega = (i, \tau)$. Since τ is now dependent on the parameter space, we must be careful with how we formulate the collision operator in order to retain mass balance. Then it is necessary to consider not the integral mass $\langle m \rangle$, but rather the weighted average $\langle \tau^{-1} m \rangle$. From a Boltzmann perspective, this corresponds to the mass (per time) entering collisions. From our perspective, this represents the mass (per time) leaving a continuum. Similarly, we are therefore also interested in not only the equilibrium distribution, but also how mass is distributed from collisions,

$$f_{i,coll}(\tau) = \frac{\tau^{-1} f_{i,eq}(\tau)}{\langle \tau^{-1} f_{eq} \rangle}. \qquad (11)$$

We will in the continuation suppress the dependence on i or τ when it is clear from the context. Motivated by this analogy to the Boltzmann equation, we will investigate a collision term of the type

$$N_{CTRW}\big(m|_{\boldsymbol{x},t}\big) = \langle \tau^{-1} m \rangle\, f_{coll}^* - \frac{m}{\tau}. \qquad (12)$$

We recognize the first term on the right hand side as the source to the continua from exchanges, while the second term represents the loss term.

Using the collision term suggested in Equation (12) in the MP model given in Equation (5), and by transforming the equation from using a fluid flux to particle velocity as parameter, so that $\boldsymbol{v}_i = (\phi\varphi_i)^{-1} \boldsymbol{u}_i$, we can write the dispersion free MP model in terms of the mass $m = m_i(\boldsymbol{x}, \tau, t)$,

$$\partial_t m + \nabla_x \cdot (\boldsymbol{v}\, m) = \langle \tau^{-1} m \rangle\, f_{coll} - \frac{m}{\tau}. \qquad (13)$$

It is convenient to change dependent variables so that Equation (13) is written in terms of the mass lost to exchange, $p_i(\boldsymbol{x}, \tau, t) = \tau^{-1} m_i(\boldsymbol{x}, \tau, t)$ in stead of the mass distribution, which

gives the equation

$$\partial_t p + \nabla_x \cdot (\boldsymbol{v}\, p) = \frac{\langle p \rangle\, f_{coll} - p}{\tau}. \tag{14}$$

This equation governs the evolution of the mass per time changing continua p, and has the same structure as the Boltzmann equation with the BGK relaxation term. This quantity is related to the *arrival* probability R solved for in the CTRW model, as we can see from Equation (12). However, Equation (14) is of a very different form than Equation (6).

We now proceed by writing Equation (14) on a Lagrangian form. By integrating Equation (14) along characteristics from time $t - \epsilon\tau$ to t, we obtain

$$p_i(\boldsymbol{x}, \tau, t) = p_i(\boldsymbol{x} - \boldsymbol{v}_i \epsilon\tau, \tau, t - \epsilon\tau) + \int_{-\epsilon\tau}^{0} N_{i,CTRW}\big(\tau\, p_i|_{\boldsymbol{x}+\boldsymbol{v}_i\tau', t+\tau'}\big)\, d\tau'. \tag{15}$$

While in general, ϵ is some small parameter, it is helpful to keep in mind the special case where $\epsilon = 1$, as this leads to needed simplifications the later expressions. This is equivalent to considering a Lagrangian step which is exactly equal to the inverse exchange rate.

To treat the integral in Equation (15), we approximate the integral by simple quadrature. Let the integral over the collision operator be approximated by its lower limit;

$$\int_{-\epsilon\tau}^{0} N_{i,CTRW}\big(\tau\, p_i|_{\boldsymbol{x}+\boldsymbol{v}_i\tau', t+\tau'}\big)\, d\tau' \approx \epsilon\tau\, N_{i,CTRW}\big(\tau\, p_i|_{\boldsymbol{x}-\boldsymbol{v}_i\epsilon\tau, t-\epsilon\tau}\big). \tag{16}$$

Then substituting the definition of the exchange term we obtain from Equation (15)

$$\begin{aligned} p_i(\boldsymbol{x}, \tau, t) &= (1 - \epsilon) p_i(\boldsymbol{x} - \boldsymbol{v}\epsilon\tau, \tau, t - \epsilon\tau) \\ &+ \epsilon\langle p \rangle(\boldsymbol{x} - \boldsymbol{v}_i\epsilon\tau, t - \epsilon\tau)\, f_{i,coll}(\tau; \boldsymbol{x} - \boldsymbol{v}_i\epsilon\tau, t - \epsilon\tau). \end{aligned} \tag{17}$$

We see that for homogeneous problems, where the exchange term is independent of space, the last term of Equation (17) is decoupled. When we chose the discretization parameter $\epsilon = 1$, the first term on the right hand side of Equation (17) is zero, which allows us to obtain an equation for the evolution of the total mass by integrating over Ω, leading to:

$$\langle p \rangle(\boldsymbol{x}, t) = \sum_i \int_0^t \langle p \rangle(\boldsymbol{x} - \boldsymbol{v}_i\tau, t - \tau)\, f_{i,coll}(\tau; \boldsymbol{x} - \boldsymbol{v}_i\tau, t - \tau)\, d\tau. \tag{18}$$

By changing the variables of integration we can go from a velocity formulation to a spatial formulation, with $\boldsymbol{x}_i' = \boldsymbol{v}_i\tau$ and $t' = \tau$.

$$\langle p \rangle(\boldsymbol{x}, t) = \sum_i \int_0^t \langle p \rangle(\boldsymbol{x} - \boldsymbol{x}_i', t - t')\, f_{i,coll}(t')\, dt'. \tag{19}$$

Here, we have assumed that the collision operator is homogeneous in space-time.

For Equation (19) to be equivalent to Equation (6), we identify the distribution ψ_{MP} as the CTRW distribution,

$$f_{i,coll}(t) = \psi_{CTRW}(\boldsymbol{x}_i, t). \tag{20}$$

We note by comparing equations (6) and (19) that the probability R of a particle arriving at a point in the CTRW model satisfies the same equation as the mass change $\langle p \rangle$ at a point in a discrete-continuous form of the MP model as given in Equation (19). For spatially discrete distributions as given in Equation (20), integration needed to convert from arrival probability R to a conservative probability P is analogous to the relationship between mass collision densities p to physical masses m. Thus we have reached the conclusion that the CTRW can be interpreted as a spatial discretization of an approximate MP model in Lagrangian coordinates, where the interaction term is evaluated by one-sided quadrature.

We summarize the relationship between the parameters of the MP and the CTRW models in Table 1, together with several of the intermediate distributions used in the derivation. The

key results are given in bold.

Property	Expression
Multiple Porosity Equation	$\partial_t m_i + \nabla_x \cdot (\rho \, \boldsymbol{u}_i \, c) = \sum_j \int_{\Omega_c} \kappa_{i,j}(\omega_c, \omega') c(\omega') \, d\omega'$
Parameter space	$\Omega = \mathbb{P} \times \mathbb{R}^+$
Parameter variable	$\omega = (i, \tau)$
Lagrangian transport kernel	$f_{i,coll}(t) = \psi_{CTRW}(\boldsymbol{x}'_i, t)$
Equilibrium distribution	$f_{i,eq}(\tau) \sim \tau \, \psi_{CTRW}(\boldsymbol{x}'_i, \tau)$
Discrete structure	$\varphi_i(\tau) \neq 0 \Rightarrow \boldsymbol{u}_i \tau = \boldsymbol{x}'_i \rho \phi \varphi_i(\tau)$
Flux density relation	$\varphi_i(\tau) = f_{i,eq}(\tau) = \tau \, \psi_{CTRW}\left(\dfrac{\boldsymbol{u}_i \tau}{\phi \varphi_i(\tau)}, \tau\right)$
Exchange term kernel	$\kappa_{i,j}(\tau, \tau') = \dfrac{1}{\tau'} \psi_{CTRW}\left(\dfrac{\boldsymbol{u}_i \tau}{\phi \varphi_i(\tau)}, \tau\right) - \dfrac{\delta(\tau - \tau')}{\tau} \delta_{i,j}$

Table 1: The main parameter functions of the MP model expressed in terms of the parameter functions of the CTRW model are give in the table in bold. Various other expressions of interest from this section are also provided.

5   EXAMPLE CALCULATION

To illustrate the relation between the parameters of CTRW and MP models we investigate a simple representation of a 2D network with a regular triangular structure. With flow aligned with the network, this network has two types of pore throats: parallel and inclined to the flow direction.

In such a synthetic case the fluid after complete mixing in a pore node will with probability $\eta_1 = 2/3$ go through the inclined pore, and with probability $\eta_1 = 1/3$ go through a parallel pore. The corresponding travel distances are denoted Δx_1 and Δx_2, with $\Delta x_2 = 2\Delta x_1$. Similarly, we denote the travel times Δt_1 and Δt_2.

Considering the described porous system in the CTRW framework we first observe that for this simple network, we only have two continua, and that the distribution of transit times is also discrete. Thus we replace the continuous time derivation from Section 4 with an equivalent discrete time random walk formulation. The transition probability is then given as

$$\psi(x'_i, t') = \begin{cases} \eta_1 & \text{if} \quad x'_i = \Delta x_1 \ \text{and} \ t'_i = \Delta t_1 \\ \eta_2 & \text{if} \quad x'_i = \Delta x_2 \ \text{and} \ t'_i = \Delta t_2 \end{cases}$$

Following the calculations in Table 1 we can rewrite the exchange term kernel on the form

$$\kappa_{i,j} = \frac{\eta_i}{\Delta t_j} - \frac{\delta_{ij}}{\Delta t_i}$$

Figure 1 shows a comparison between the break-through curves obtained by a network model as described, together with the equivalent dual-porosity model. The parameters have been chosen to be characteristic of homogeneous sand. While this is a relatively simple problem, the example nevertheless validates the connection between CTRW and MP models derived in Section 4. We also note that for these parameters, even though the coupling term κ is relatively strong, the curves nevertheless show a devitation from the error function predicted by a single porosity model.
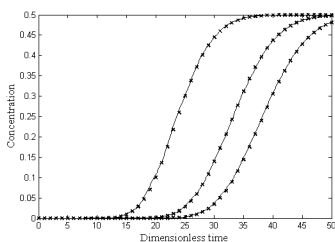

Figure 1. Concentration profiles obtained different distances from the injection point. Results from network model (lines) and dual-porosity model (crosses).

5   DISCUSSION

We summarize the main results and observations herein:
1. Given a suitable approximate Lagrangian form, the parameters of the multiple porosity model can be obtained from the parameters of the continuous time random walk model.
2. Conversely, the continuous time random walk model can be seen as a spatial discretization of an approximate Lagrangian form of the multiple porosity model.
3. A suitable interpretation of the different continua in the multiple porosity model is that they represent fluxes and expected particle travel times between change in flux field.
4. The kernel κ of the exchange transform can be expressed explicitly given the flux density φ.
5. In practice, only a (small) finite number of continua are used in multiple porosity models. The multiple porosity model can then be seen as a flux space discretization of the underlying transition time distribution ψ, as opposed to continuous time random walk which is a spatial discretization.

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