Solute Dispersion by 1D Stepped Velocity Fluctuations

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Abstract: The effect of fluctuations in the drift velocity on dispersion by a porous medium is investigated. An analytical model is developed which represents the effect of a single discrete step in the velocity of a 1-dimensional flow as a multiplicative factor that modifies the underlying linear growth in solute variance predicted by the standard advection-dispersion equation. The algebraic structure of the model identifies two variable combinations Δ and α that characterize the step and the rate of stochastic dispersion respectively, in terms of which a simple formula for the downstream effect of the step on dispersion is obtained. This formalism is next applied to a sequence of 3 steps representing a velocity fluctuation, and it is shown that while kinetic compression effects cancel out across such a fluctuation, the stochastic dispersion increases for any plausible combination of Δ and α. This implies that a dispersion enhancement factor f is associated with a fluctuation, and a simple formula is obtained for this in terms of variables that describe the fluctuation length and amplitude. Moreover, the algebra leads to the definition of a natural length scale Λ related to the Peclet number of the flow. Repeated application of this formula is used to find the cumulative dispersion enhancement by a sequence of identical fluctuations, leading to an expression for dispersivity as a function of the distance traversed by a solute plume. Key features of the model are that the dispersivity behaves differently for traversal lengths above and below Λ, and that above this transition it is proportional to a fractional power of the traversal length. These features are in agreement with experimental observation of scale-dependent dispersivity, but quantitatively the observed growth in dispersivity over several orders of magnitude is not obtained for any reasonable choice of parameter values.

Keywords: Solute dispersion; dispersivity; velocity fluctuations; stochastic modeling; scale-dependent.

1. INTRODUCTION

It is a well-known fact [Fetter (1999)] that the observed dispersivity of natural porous media such as underground aquifers depends strongly on the length scale of the flow for which dispersion is measured. It is also widely accepted that this is related to the inhomogeneity of natural media, i.e. variations in the hydraulic conductivity and porosity of such media.

This paper presents a further step in our ongoing investigation of this phenomenon, that is based on the premise that variations in media properties and geometry cause macroscopic variations in the drift velocity of the fluid that carries a solute plume through the medium.

Such variations have been shown previously to modify the diffusion-like behavior of dispersion in a constant flow velocity. Diffusive behavior (as follows from Fick's law) is exemplified by the linear time-dependence of a gaussian concentration plume variance with initial value S^2

$$\sigma^2(t) = S^2 + 2Dt \qquad (1)$$

where $D = d\,v$ is defined as the dispersion coefficient, d as the dispersivity and v is the constant drift velocity.

In particular, we have shown [Kulasiri and Verwoerd (2002)] that if v changes linearly with the traversal length x of the plume, an exponential increase or decrease of the variance with time replaces the linear growth. Part of this is merely a reversible kinematical effect, but there is also an irreversible part that expresses an interaction between random deflections of the fluid flow by the pore structure, and a macroscopic change of the flow velocity v. This interaction is a consequence of the fact that at a microscopic level, the motion of fluid elements is described by a stochastic partial differential equation (SPDE) in which v plays the role of a driving coefficient.

A similar but less dramatic deviation from linear diffusive behavior has also been demonstrated [Verwoerd and Kulasiri (2001)] for the discrete velocity steps of a piecewise constant, 1-dimensional velocity. In this case it was found that when a gaussian concentration plume propagates through a step, the profile remains approximately gaussian but the variance is now given by the expression:

$$\sigma^2(t) = \frac{\gamma^2(t - t_c)}{a(T)}; \qquad t_c = \frac{-S^2}{\gamma^2} \qquad (2)$$

For a constant velocity $a(T) = 1$ and we recover the linear time relationship. In this equation γ is

the amplitude of the stochastic term in the underlying SPDE, and a comparison of equation (2) in the constant velocity case with equation (1) shows that apart from proportionality constants γ^2 then reduces to the dispersion coefficient D

The most significant feature of equation (2) is that beyond a step, the linear time dependence is modified by the multiplicative factor $1/a(T)$. Here T is a dimensionless time parameter expressed in terms of the time θ at which the plume reaches the step, and $a(T)$ is approximated by

$$a(T) = 1 - \frac{4\alpha^2 \Delta}{T^2 (\alpha + \Delta)^2} \qquad (3)$$

Here $\Delta = (V_2 - V_1)/(V_2 + V_1)$ is a dimensionless parameter that characterizes the height of the velocity step from V_1 to V_2, and α is the ratio of the plume variances at the entry and exit points of the velocity regime that is terminated at the step under consideration. The approximation holds for $\Delta < 0.3$.

When the peak reaches the step, $T = 1$. In the absence of dispersion $\alpha = 1$ and then $a(1)$ reduces to the kinematical value $(1-\Delta)^2/(1+\Delta)^2$. With dispersion, equation (3) only applies at T sufficiently larger than 1 that the plume has fully penetrated the step. At such a time a(T) approaches the kinematical compression (stretching) of the plume at a downwards (upwards) velocity step, but then decays back to a value of 1 for large times (i.e., at positions far beyond the step).

The cases of linear velocity growth over an indefinite period, and of a velocity step, both demonstrate the principle of non-linear dispersion growth, but neither represents a realistic scenario. Instead, an actual flow through an aquifer would be expected to show fluctuations of the flow velocity around the average that is deduced from total flow volume measurements.

To model that, this paper sets out to explore the extension of the single step results to multiple steps, such as may be used to describe a series of fluctuations of the flow velocity about an average value. Clearly such a piecewise constant velocity description is still highly idealized, but has the advantage that with a simple formula such as equation (3) it is feasible to perform a detailed calculation analytically and hence gain far more insight into the important processes and variables that are involved.

2. THE MULTIPLE STEP MODEL

In the detailed analysis of the single step, it was found that a gaussian incident concentration peak is somewhat distorted when it penetrates the step, and this was expressed by a slowly varying modulation factor that multiplies the transmitted peak. As a simplifying assumption, we now ignore the modulation and hence use the output gaussian, with its non-linear time dependent variance, as the input gaussian for the next step.

The variables that are needed to describe the effect of the m-th step are then given by the following expressions:

$$T_m = \sqrt{\frac{t - t_c}{\theta_m - t_c}} \; ; \qquad \alpha_m = \frac{\theta_m - t_c}{\theta_{m-1} - t_c} \qquad (4)$$

In a similar way Δ acquires an index and is calculated by appropriately assigning the applicable velocity values for the particular step.

While the output gaussian from step m propagates to step $(m+1)$, its variance changes and so the input variance for step $(m+1)$ is found by evaluating equation (3) for $a_m(T_m)$ at the T_m-value obtained by setting $t = \theta_{m+1}$, hence reducing T_m to $\sqrt{\alpha_{m+1}}$. When the peak emerges from step $(m+1)$, the variance acquires an additional factor $1/a_{m+1}(T_{m+1})$ which once more is evaluated at $T_{m+1} = \sqrt{\alpha_{m+2}}$ to give the input gaussian for step $(m+2)$.

In this way the cumulative effect of a sequence of M steps, is to multiply the variance by an enhancement factor F_M defined by using eq (3) as:

$$F_M = \prod_{m=1}^{M} \frac{\alpha_{m+1}(\alpha_m + \Delta_m)^2}{\alpha_{m+1}(\alpha_m + \Delta_m)^2 - 4\alpha_m^2 \Delta_m} \qquad (5)$$

In this expression, strictly speaking the M-th factor and hence also F_M should still be a function of an undetermined T_M-parameter. But in most applications one envisages an infinite sequence of steps and M is simply the number of steps that the plume has penetrated in moving from the origin to a position x. Then it is appropriate to evaluate the effect of the first M steps at the time when it enters the $(M+1)$-th, and equation (5) is obtained.

As a simple illustration of the use of this formula, suppose that a smooth linear velocity growth v = v_0 + p x , is approximated by a "staircase" of regularly spaced small discrete steps, all with the same value for Δ. In this case, the relation between the continuous and stepped versions is expressed by

$$M = \left(\tfrac{1+\Delta}{2\Delta}\right) p t \qquad (6)$$

where t is the time at which the plume reaches x.

Suppose first that there is no dispersion, i.e. the deterministic limit, and so all $\alpha = 1$. Then the product expression becomes a simple power law

$$F_M = \left(\frac{1+\Delta}{1-\Delta} \right)^{\frac{1+\Delta}{\Delta} pt} \qquad (7)$$

and in the limit of large M, i.e. small Δ, this reduces to e^{pt} by virtue of the well known identity $(1+\frac{x}{n})^n \xrightarrow[\infty]{n} e^x$. This exponential growth or decline is identical to that calculated directly for the deterministic evolution of a gaussian plume in a flow with a constant velocity gradient p.

Returning to the full dispersion expression, the θ_m may be expressed in terms of Δ and p and used to substitute the α_m in equation (5). The resulting product is complicated but may be expressed in terms of Gamma-functions, and these approximated by the Stirling approximation. In this way similar exponential factors as for the deterministic case are retrieved. Again the result can be compared to the exact result derived [Kulasiri and Verwoerd (2002)] for stochastic dispersion in a constant velocity gradient. The analytical expressions are in this case not identical, as a result of the approximations involved in equation (3), but contain similar exponential terms and give a very similar numerical behavior.

The success achieved in using the discrete step approach as a model in the case of a linear velocity change for which exact results are known, gives us confidence to apply the same approach to model the as yet unknown case of velocity fluctuations.

The decay of the single step factor in equation (3) beyond the step position implies that there is an associated length scale. Length scale effects are bound to follow from this for fluctuations made up of steps. It is therefore prudent to construct the fluctuation model in such a way that it has a unique characteristic length, allowing analysis of how this length affects the final results. That is most easily achieved by locating all steps at the positions of a fixed periodic grid, with a spacing L. Figure 1 illustrates the simple fluctuation model assumed for the work presented here.

The value V represents the average flow velocity. The value of V_2 is fixed by freely choosing the step size parameter Δ to determine the amplitude of the fluctuation about V; i.e., $V_2 = V(1+\Delta)/(1-\Delta)$. Then V3 is chosen in such a way that the average velocity will indeed be V, and this is found to be $V_3 = V(1+\Delta)/(1+3\Delta)$. So the fluctuations are fully characterized by the amplitude parameter Δ and the fluctuation length 3L which is in effect the periodic repeat length.
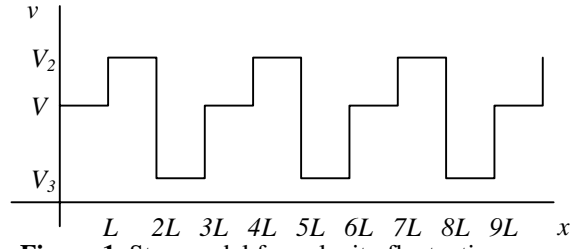
Figure 1. Step model for velocity fluctuations on a periodic grid of length L

In the absence of dispersion, the only effects of the steps are the kinematical compression or stretching of the gaussian solute peak required by flux conservation, and these obviously cancel over the combination of 3 steps that make up a single fluctuation. It therefore makes sense to also collect the 3 steps together when describing the evolution of the plume in the presence of dispersion. Any deviation from 1, in the combined multiplicative factor, can then clearly be ascribed to a fluctuation effect on dispersion.

The first step in this calculation is to find the arrival times of the peak at each step, as $\theta_i = \Theta_i(L/V)$ where the dimensionless arrival times Θ_i are $\Theta_1 = 1$, $\Theta_2 = 2/(1+\Delta)$ and $\Theta_3 = 3$. Putting these into the definitions of the α_i as in equation (4) we find

$$\alpha_i = \frac{\Theta_i - \frac{V t_c}{L}}{\Theta_{i-1} - \frac{V t_c}{L}} \qquad (8)$$

This equation exhibits a crucial fact that pervades all of the results on the fluctuation model, namely that all lengths are measured with respect to a common length scale defined by

$$\Lambda = -V t_c = V S^2 / \gamma^2 \qquad (9)$$

This is applied by replacing L in the expression for the Θ_i by the scaled grid spacing $\lambda = L/\Lambda$

The effect of the first fluctuation that the plume encounters is then given by an enhancement factor $f = F_3$ in the notation of equation (5), and it is easily seen that this is a function of only the two dimensionless parameters Δ and λ that characterize the fluctuation amplitude and length respectively.

The analytical form obtained for $f(\lambda, \Delta)$ is very complicated, but its numerical behavior is rather simple, as shown in figure 2. Plausibly, for either $\Delta = 0$ or $\lambda = 0$, $f = 1$ and there is no enhancement.
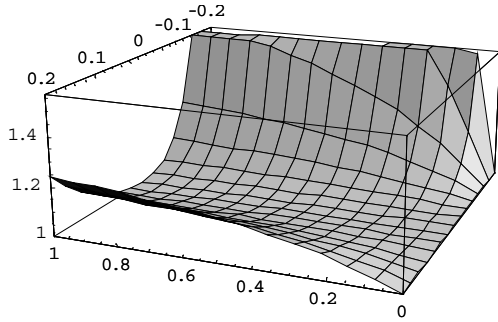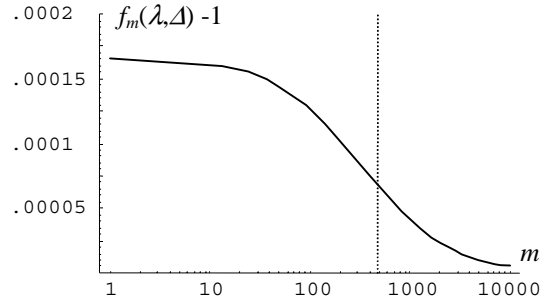
Figure 2. The single fluctuation enhancement factor for $-0.2 < \Delta < 0.2$, and $0 < \lambda < 1$.

However, a very significant feature seen in the figure is that for all other combinations of Δ and λ values, f is greater than 1, which means that dispersion is *increased* relative to the diffusive or Fickian values by a fluctuation. It is not obvious that this will happen, as a single upwards velocity step suppresses dispersion while a downwards step increases it, and without dispersion these effects cancel exactly across a fluctuation. We have earlier shown [Verwoerd and Kulasiri (2001)] from numerical calculations that a net residual enhancement of dispersion across a fluctuation is obtained for a specific example, but the analytical result reported here is a major advance as it shows that this is true in general. The parameters displayed in the figure cover a generous range, allowing for the maximum and minimum velocities to differ by $\approx$40% from the average, and as will be seen below only $\lambda \ll 1$ is expected to be physically relevant.

This result adds substantially to the plausibility of the simplified model under discussion where all fluctuations are assumed to be identical. If f turned out to be <1 for some fluctuations, it might have been argued that in a realistic system fluctuations over a range of amplitudes and lengths will be present and could cancel each other. As this is not the case, the present model where in effect the ranges are represented by their averages and the effects from subsequent fluctuations are allowed to accumulate, appears quite reasonable as a first approximation.

The next step is to include multiple fluctuations in the calculation. We modify the notation slightly in henceforth using m as an index counting fluctuations rather than steps. Equation (5) is accordingly modified by replacing the single step factor that appears as the subject of the product, by a product of the 3 step factors that make up the m-th fluctuation. Analytical calculation of this single fluctuation enhancement factor $f_m(\lambda,\Delta)$ proceeds as outlined above for the special case now written as $f_1(\lambda,\Delta)$. Once more a very

complicated, but rational algebraic expression is obtained for $f_m(\lambda,\Delta)$. The nature of its m-dependence is illustrated in figure 3.

Figure 3. Dependence of the single fluctuation enhancement (solid line) on the fluctuation number m, for $\Delta = 0.1$ and $\lambda = 0.001$. The dotted line corresponds to the scale length Λ .

The enhancement encountered by the plume as it traverses a sequence of fluctuations decreases slowly at first, but when it reaches the m-value that corresponds to the scale length Λ there is a sharp decline and a further asymptotic decrease beyond that. The parameter values chosen to display this behavior, were found by taking a Peclet number between 1 and 10, the initial plume extension of the order of 10^{-2} m and the pore diameter 10^{-4} m. These are merely meant as plausible order of magnitude estimates and lead to a Λ value in the order of 10 m or larger. Then the assumed value $\lambda = 0.001$ implies a physical fluctuation length of about 3 cm, which appears a reasonable estimate of the scale on which inhomogeneities appear in natural aquifers.

The crucial role played by Λ is seen to be as a *transition point* between distinct short range and long range behaviors of the enhancement factor. Such a distinction between short- and long range behaviors is also noticeable in experimental observations of the dispersivity that extend over a sufficient spatial scale, and it is gratifying to find it arising as a natural consequence of the mathematics of the fluctuation model.

However, before dispersivity can be calculated, it is first necessary to perform the repeated product of enhancement factors required by equation (5). Unfortunately, this is not feasible with the complicated form obtained for f_m so far and we resort to an approximate expression for it.

The strategy used to find such an approximation, is to make three series expansions of f_m about the points $m = \infty$, $\lambda = 0$ and the point $m = 1/2\lambda$ that falls inside the transition range; then a simple function was guessed that has the same

dominating terms in its series expansions about the same points. A surprising feature of the dominating terms in all three expansions is that the Δ-dependence is separated out into an identical rational polynomial expression that we designate as $Q(\Delta)$. In terms of this the approximation found is

$$f_m(\Delta,\lambda) \approx \frac{3\lambda\, Q(\Delta)}{1+3m\lambda} \qquad (10)$$

This amazingly simple expression reproduces the behavior of the full formula for f_m to such an extent that it is indistinguishable from the original curve for the parameter values shown in figure 3; only when λ approaches 1 does it underestimate the exact value by a few percent in the low range, while the high range values are still very close.

A plot of the Q function for a range of Δ-values is shown in figure 4.
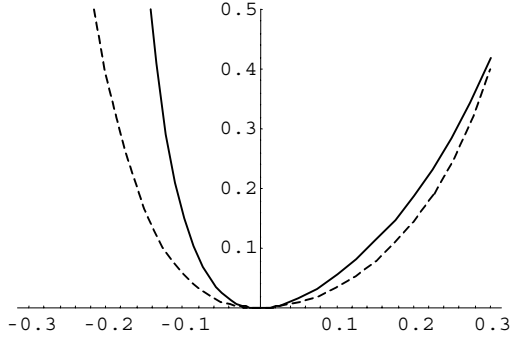
Figure 4. Q as a function of step size parameter Δ, for the regular grid fluctuation model (solid line) and for a non-grid model (dashed line).

The calculations described so far have also been done for a slightly more general fluctuation model, in which the restriction of steps to lie at grid points was relaxed. It turns out that while the full expression for f_m is different, equation (10) still holds but a somewhat different expression for $Q(\lambda)$ is obtained. Both curves are plotted in figure 4, and while Q is seen to be moderately sensitive to the details of the shape of the assumed fluctuation profile, Q values are less than about 0.4 for reasonable fluctuation amplitudes.

Equation (10) is simple enough that when substituted into equation (5) the expression for the cumulative enhancement factor F_M can be calculated analytically. It is obtained as a ratio of two Pochhammer functions which are themselves defined as a ratio of Gamma functions. The Stirling approximation is applied to these, and after simplification we obtain the following

expression for the cumulative enhancement factor:

$$F_M = \left(1+\frac{3Q\lambda}{3M\lambda+1}\right)^{M}\left(1+\frac{3M\lambda}{3Q\lambda+1}\right)^{Q} \times$$
$$\times\left(1-\frac{9MQ\lambda^2}{(3M\lambda+1)(3Q\lambda+1)}\right)^{\frac{1}{2}+\frac{1}{3\lambda}} \qquad (11)$$

When the plume has traversed a distance x, the number M of fluctuations that it has encountered is given by $x = 3LM$ and the time t taken is $x = Vt$.

One way to proceed is to eliminate M in favor of t, and then multiply this by the diffusive dispersion expression $\gamma^2(t-t_c)$ of equation (2) to get the gaussian variance of the plume. This is clearly non-linear in t and a commonly used strategy is to take the time derivative of that as the dispersion coefficient D. On the other hand, one may simply take the D as the coefficient of the factor $(t-t_c)$, i.e. divide the variance expression by $(t-t_c)$ instead of differentiating it. Both procedures give the same result in the only case where the definition of a dispersion coefficient is strictly meaningful, i.e. the case of diffusive dispersion. Non-linear time dependence of the variance gives a slightly different result, but the division procedure that in effect extracts an average value over the interval $(0,t)$, is closer to the way dispersivity is determined experimentally.

We therefore use the latter method, and in the present context, finding the dispersivity then reduces to simply multiplying the calculated enhancement factor by a constant, namely the initial (laboratory scale) dispersivity. In other words, the enhancement factor F can be considered as merely the (dimensionless) scaled dispersivity. As the measured values are expressed as a function of the traversal length x rather than time t, we eliminate M in equation (11) in favor of the scaled traversal length $\Gamma = x/\Lambda$ by the relation

$$\Gamma = 3\lambda M \qquad (12)$$

The resulting behavior of $F(\Gamma)$ is shown in figure 5, over 5 orders of magnitudes of the traversal length, similar to the range of experimental values collected by Gelhar (1986) and further analysed by Fetter (1999). The figure shows that there is a distinct transition from a low range behavior to a high range behavior when the traversal length reaches the scale length Λ. Such a transition is also seen in the experimental values, at a length of between 10 and 100 meters.
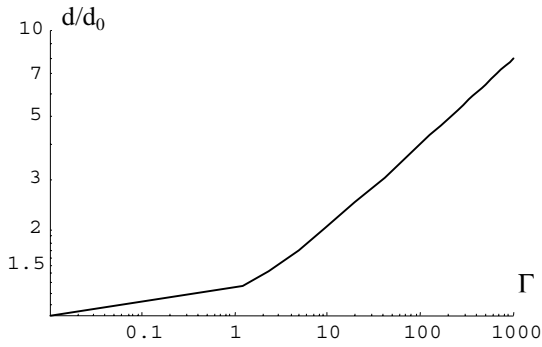
Figure 5. Logarithmic plot of scaled dispersivity as a function of scaled traversal length for $\lambda = 0.001$ and $Q = 0.3..$

The high range behavior is easily extracted from the analytic expression in equation (11) by taking the large M limit, as M is proportional to Γ. In this limit the first factor reduces to e^Q (a constant) and the last factor also becomes constant, so that the entire Γ-dependence is carried by the second factor which simplifies to $(1+\Gamma)^Q \rightarrow \Gamma^Q$. This power law becomes a straight line with slope Q in the logarithmic plot, which agrees with the observed high range behavior. Even more significant, the measured values suggest a slope of approximately 0.3, and this agrees with the restricted range of Q values derived from the mathematical properties of the fluctuation model as shown in figure 4.

However, there are also two points on which figure 5 differs markedly from the observations. First, the low range trend in the figure is a slower rate of growth than in the high range while the reverse holds for the measurements. Secondly, as a result of this the overall increase in the figure is only by a factor of 10 , while an increase of 10^4 is found for measured values.

This vast numerical discrepancy hinges on a single detail of the low range behavior. For $\Gamma<<1$ i.e. $M << 1/3\lambda$, the increase of F with Γ is dominated by the first factor in equation (11), and this increases roughly exponentially with Γ. At the transition point it saturates to the value e^Q and with any reasonable value of Q this is far too small to produce the observed rise of 3 orders in magnitude in dispersivity up to the transition.

The simple ad hoc change of increasing the coefficient of Q in the first term of equation (11) by a factor of about 25 is found to remove both discrepancies and give a dispersivity curve in rather good agreement with the experimental values. However, there is no obvious justification for such a change within the confines of the stepped fluctuation model presented, and further investigation of this point is left to our subsequent paper.

3. CONCLUSIONS

The model using fluctuations formed from 1-dimensional discrete velocity steps on a regular grid to describe longitudinal dispersivity, is no doubt highly idealized. It can come as no surprise that full numerical agreement with observations in natural aquifers is not obtained. In fact, in view of additional effects bound to appear in higher dimensional systems complete agreement would have been questionable.

However, the model amply demonstrates how minor enhancement effects of individual fluctuations on solute dispersion, can combine to create the complex dependence of dispersivity on measurement scale that is observed, as well as the dramatic magnitude of these effects. At root, this is because of the multiplicative way that enhancements combine, a result that is expected to transcend the details assumed for fluctuations.

Moreover, the level of agreement is sufficient to suggest that the model has captured the essential underlying mechanism of scale dependence. In particular, the identification of a macroscopic length scale that dictates the phenomenon, is a significant new concept.

Finally, the feasibility of algebraic analysis brought about by the relative simplicity of the model, allows significant variables and combinations of variables to be identified. For example, the result that the fluctuation amplitude represented by $Q(\Delta)$ uniquely determines the long range behavior of the dispersivity, is a sufficiently general and qualitative statement that it should be amenable to direct experimental testing or comparison with other theories.

4. REFERENCES

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