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Calculating how long it takes for diffusion processes to reach steady state: application to groundwater flow

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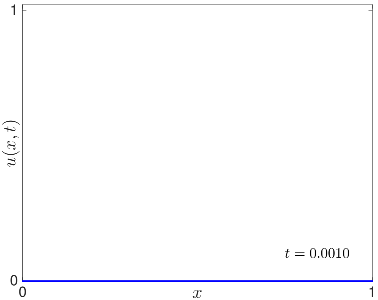
Mathematical problem

- How long does a diffusion process take?

$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial x}\left(D(x)\frac{\partial u}{\partial x}\right), \quad 0 < x < L.$$



- Finite transition time:

$$\frac{u(x,t_s) - u_\infty(x)}{u_0(x) - u_\infty(x)} = \delta$$

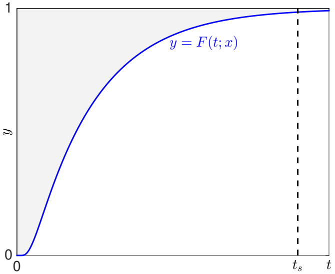
Mean action time (MAT) approach

- Transition can be represented as a CDF:

$$F(t;x) := 1 - \frac{u(x,t) - u_\infty(x)}{u_0(x) - u_\infty(x)}$$

- Equivalently, finite transition time satisfies:

$$F(t_s;x) = 1 - \delta$$

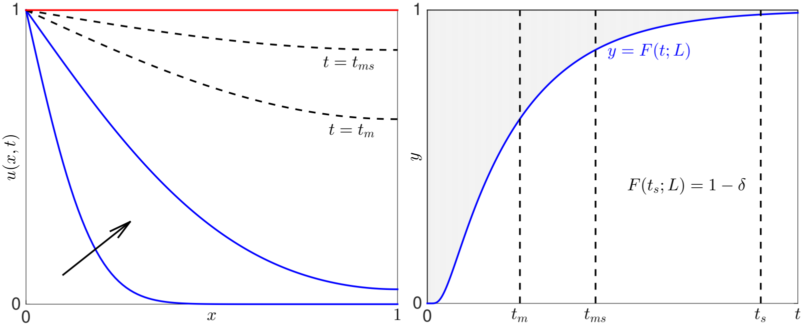


- *Mean action time*: common measure of the time required to reach steady state[1]

$$\mathrm{MAT}(x) := M_1(x) = \int_0^\infty t f(t;x)\,\mathrm{d}t; \quad f(t;x) = \frac{\partial F}{\partial t}(t;x).$$

[1] McNabb and Wake (1991); Landman and McGuinness (2000); Simpson et al. (2013)

Mean action time (MAT) approach



$$t_m := \mathrm{MAT}(L) = M_1(L)$$

$$t_{ms} := (\mathrm{MAT} + \sqrt{\mathrm{VAT}})(L) = M_1(L) + \sqrt{M_2(L) - M_1^2(L)}$$

Computing the moments

- kth raw moment

$$M_k(x) = \int_0^\infty t^k f(t;x)\,\mathrm{d}t,$$
$$f(t;x) = \frac{1}{u_\infty(x) - u_0(x)} \frac{\partial}{\partial t}\left[u(x,t) - u_\infty(x)\right].$$

- Boundary value problem for scaled moment $\overline{M}_k(x) = M_k(x)(u_\infty(x) - u_0(x))$[2]:

$$\frac{\mathrm{d}}{\mathrm{d}x}\left(D(x)\frac{\mathrm{d}\overline{M}_k}{\mathrm{d}x}\right) = -k\overline{M}_{k-1}(x), \quad 0 < x < L,$$
$$\overline{M}_k(0) = 0, \quad \frac{\mathrm{d}\overline{M}_k}{\mathrm{d}x}(L) = 0.$$

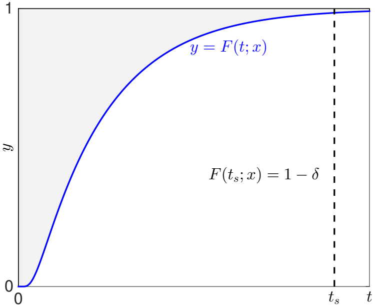
- Recursively solve boundary value problems. Starting with $k = 1$ and given $\overline{M}_0(x) = u_\infty(x) - u_0(x)$. Repeat until a desired order.

[2] Carr (2017)

Calculating the transition time

- Transient solution has functional form:

$$u(x,t) = u_\infty(x) + \sum_{n=1}^{N} c_n e^{-t\beta_n}$$



- Follows that:

$$F(t;x) = 1 - \frac{u(x,t) - u_\infty(x)}{u_0(x) - u_\infty(x)}$$
$$= 1 - \sum_{n=1}^{N} \alpha_n e^{-t\beta_n}$$
$$\simeq 1 - \alpha_1 e^{-t\beta_1}, \quad \text{for large } t$$

- Asymptotic estimate of finite transition time:

$$1 - \alpha_1 e^{-t_s\beta_1} \simeq 1 - \delta \quad \Rightarrow \quad t_s \simeq \frac{1}{\beta_1}\log\left(\frac{\alpha_1}{\delta}\right)$$

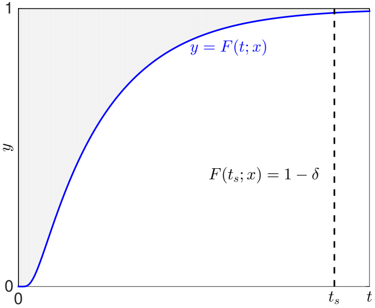
Calculating the transition time

- Transient solution has functional form:

$$u(x,t) = u_\infty(x) + \sum_{n=1}^{N} c_n e^{-t\beta_n}$$

- Follows that:

$$\begin{aligned} F(t;x) &= 1 - \frac{u(x,t) - u_\infty(x)}{u_0(x) - u_\infty(x)} \\ &= 1 - \sum_{n=1}^{N} \alpha_n e^{-t\beta_n} \\ &\simeq 1 - \alpha_1 e^{-t\beta_1}, \quad \text{for large } t \end{aligned}$$



- Asymptotic estimate of finite transition time:

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Calculating the transition time

- Asymptotic relation:

$$M_k(x) \simeq k!\frac{\alpha_1}{\beta_1^k} \quad \text{for large } k.$$

- Matching moments:

$$\begin{aligned}(k-1)!\frac{\alpha_1}{\beta_1^{k-1}} &\simeq M_{k-1}(x)\\ k!\frac{\alpha_1}{\beta_1^k} &\simeq M_k(x)\end{aligned} \quad\Rightarrow\quad \begin{aligned}\alpha_1 &\simeq \frac{M_k(x)}{k!}\left(\frac{kM_{k-1}(x)}{M_k(x)}\right)^k\\ \beta_1 &\simeq \frac{kM_{k-1}(x)}{M_k(x)}\end{aligned}$$

- Finite transition time estimate:

$$t_s \simeq \frac{M_k(x)}{kM_{k-1}(x)}\log\left[\frac{M_k(x)}{k!\,\delta}\left(\frac{kM_{k-1}(x)}{M_k(x)}\right)^k\right]$$

- No need for transient solution $u(x,t)$!

Application to groundwater flow

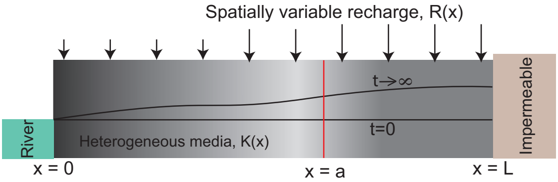

Figure 1: Simpson et al. (2013)

$$S\frac{\partial h}{\partial t} = \frac{\partial}{\partial x}\left(K(x)\overline{h}\frac{\partial h}{\partial x}\right) + R(x), \quad 0 < x < L, \;\; t > 0,$$

$$h(x,0) = h_0(x), \quad h(0,t) = h_1, \quad \frac{\partial h}{\partial x}(L,t) = 0,$$

$\overline{h}(x,t)$: saturated thickness
$K(x)$: saturated hydraulic conductivity
$R(x)$: recharge rate

Laboratory-scale aquifer model

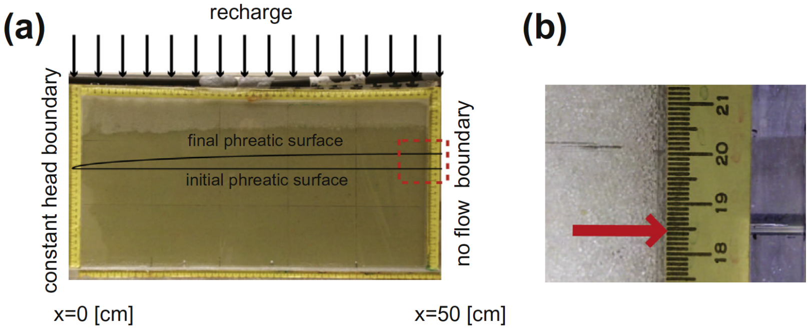

Figure 2: Simpson et al. (2013)

Results: Comparison to data

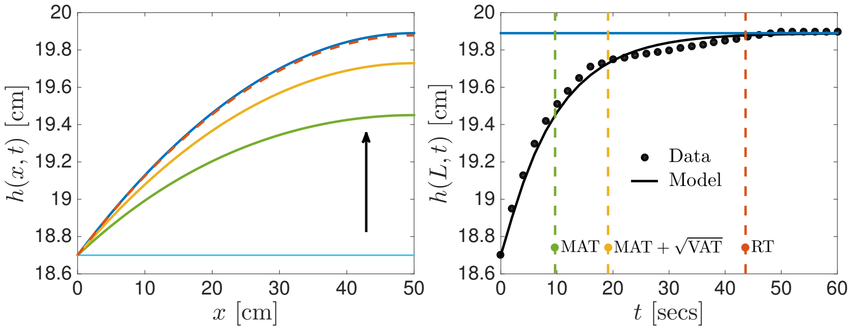

Figure 3: Carr and Simpson (2018)

How many moments are required?

	t_s	δ_s	$\lvert\delta_s - \delta\rvert$
$\mathrm{MAT}(L)$	9.6751	0.37	3.6e-01
$(\mathrm{MAT} + \sqrt{\mathrm{VAT}})(L)$	19.1152	0.14	1.3e-01
$k = 1$	44.5556	0.01	9.3e-04
$k = 2$	43.7157	0.01	8.5e-05
$k = 3$	43.6410	0.01	6.0e-06
$k = 4$	43.6356	0.01	2.3e-07
$k = 5$	43.6353	0.01	2.4e-08
$k = 6$	43.6354	0.01	8.3e-09
$k = 7$	43.6354	0.01	1.5e-09
$k = 8$	43.6354	0.01	2.4e-10
$k = 9$	43.6354	0.01	3.4e-11
$k = 10$	43.6354	0.01	4.7e-12

Table 1: Carr and Simpson (2018)

$$\delta_r = \frac{h(L,t_s) - h_\infty(L)}{h_0(L) - h_\infty(L)}; \quad t_s \simeq \frac{M_k(x)}{kM_{k-1}(x)} \log\left[\frac{M_k(x)}{k!\,\delta}\left(\frac{kM_{k-1}(x)}{M_k(x)}\right)^k\right].$$

Journal papers

PHYSICAL REVIEW E **96**, 012116 (2017)

Calculating how long it takes for a diffusion process to effectively reach steady state without computing the transient solution

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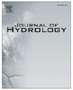

Research papers

Accurate and efficient calculation of response times for groundwater flow

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Conclusions and Summary

- Extended the mean action time concept
- New method for calculating highly accurate finite transition times using higher-order moments
- New estimate is significantly more accurate than existing estimates
- Requires significantly less computational cost than using the transient solution with standard time-stepping schemes
- Techniques presented carry over to two and three dimensional problems

References

Carr, E. J. (2017). Calculating how long it takes for a diffusion process to effectively reach steady state without computing the transient solution. *Phys. Rev. E*, 96:012116.

Carr, E. J. and Simpson, M. J. (2018). Accurate and efficient calculation of response times for groundwater flow. *J. Hydrology*, to appear.

Jazaei, F., Simpson, M. J., and Clement, T. P. (2014). An analytical framework for quantifying aquifer response time scales associated with transient boundary conditions. *J. Hydrology*, 519:1642–1648.

Landman, K. and McGuinness, M. (2000). Mean action time for diffusive processes. *J. Appl. Math. Decision Sci.*, 4(2):125–141.

McNabb, A. and Wake, G. C. (1991). Heat conduction and finite measures for transition times between steady states. *IMA. J. Appl. Math.*, 47:193–206.

Simpson, M. J., Jazaei, F., and Clement, T. P. (2013). How long does it take for aquifer recharge or aquifer discharge processes to reach steady state? *J. Hydrology*, 501:241–248.

Heterogeneous results

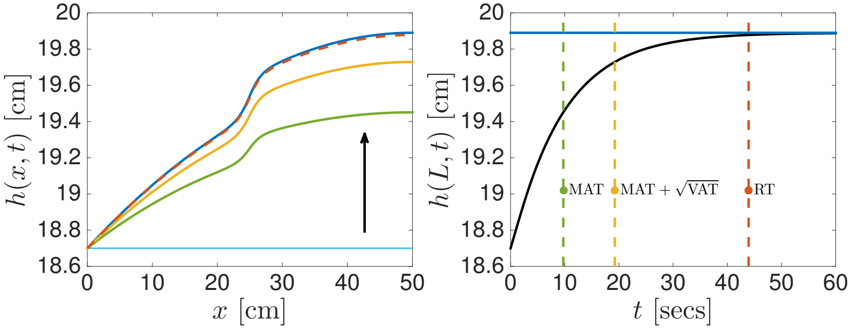

Figure 4: Carr and Simpson (2018)