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TITLE: MODIFICATIONS TO THE CONDUIT FLOW PROCESS MODE 2 FOR MODFLOW-2005

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Abstract:

As a result of rock dissolution processes, karst aquifers exhibit highly conductive features such as caves and conduits. Within these structures groundwater flow can become turbulent and thus be described by nonlinear gradient functions. Some numerical groundwater flow models explicitly account for pipe hydraulics by coupling the continuum model with a pipe network that represents the conduit system. In contrast, the Conduit Flow Process Mode 2 (CFPM2) for MODFLOW-2005 approximates turbulent flow by reducing the hydraulic conductivity within the existing

linear head gradient of the MODFLOW continuum model. This approach reduces the practical as well as numerical efforts for simulating turbulence. The original formulation was for large pore aquifers where the onset of turbulence is at low Reynolds numbers (1 to 100) and not for conduits or pipes. In addition, the existing code requires multiple time steps for convergence due to iterative adjustment of the hydraulic conductivity. Modifications to the existing CFPM2 were made by implementing a generalized power function with a user-defined exponent. This allows for matching turbulence in porous media or pipes and eliminates the time steps required for iterative adjustment of hydraulic conductivity. The modified CFPM2 successfully replicated simple benchmark test problems.

Introduction

Commonly, groundwater flow is assumed to be slow and laminar. Therefore, linear equations like those from Darcy (1856) are generally applied. Frequently used numerical groundwater flow models like MODFLOW-2005 (Harbaugh 2005) consider laminar flow only. However, rapid turbulent flow can occur through highly conductive underground structures like preferential flow layers with vuggy porosity (Shoemaker et al. 2008a, 2008b; Kuniansky et al. 2008) and the impact of these turbulent flow processes can be considerable, for example when spring flow needs to be simulated reliably to monitor adherence to minimum flow goals by water resource managers (Scanlon et al. 2003; Jeannin 2001).

Commonly, turbulent flow is described by the Forchheimer equation (Forchheimer 1901), which can be generalized to the following power law (Muskat 1946):

$$I = \frac{\partial h}{\partial x_i} = \alpha q_i + \beta q_i^m \quad (1)$$

where $I = \frac{\partial h}{\partial x_i}$ is the dimensionless hydraulic gradient, α and β are dimensionless constants related to fluid and rock properties, q_i is specific discharge [LT^{-1}], and *m* represents a constant exponent for the power law. For turbulent flow, the linear term in Equation 1 becomes small and generally can be neglected. The exponent *m* is assumed to take values between 1 and 2 (cf. Şen 1995), where *m* = 1 agrees with the Darcy equation and *m* = 2 corresponds to the Forchheimer equation and yields a discharge equal to the commonly used nonlinear flow laws, e.g. the Manning equation for free-surface flow or the Colebrook-White formula for pipe flow (Young et al. 2004). It follows that the flow exponent *m* may be interpreted as alignment for the impact of turbulence.

One feasible way to consider turbulent flow processes in karst conduits is the use of hybrid models. Hybrid models couple a discrete pipe network, where laminar and turbulent flow can occur, to a continuum model, which represents the matrix (Király 1984; Liedl et al. 2003; Shoemaker et al. 2008a). Water transfer between both compartments is realized by linear head-dependent flux. However, hybrid models require a large amount of additional data and are computationally much more complex and demanding, which constrains their widespread use.

A promising new approach is the Conduit Flow Process Mode 2 (CFPM2), a continuum model, which can be used to compute laminar or turbulent flow in large pore aquifers where the onset of turbulence is at low Reynolds numbers (1 to 100) (Shoemaker et al. 2008a, 2008b; Kuniansky et al. 2008). Because the solvers for MODFLOW sometimes use only head closure and not flow closure, and the turbulent conductance is now a function of head, the solution may not converge on a single time step. Multiple time steps are required for flow convergence with the original CFPM2. Thus, we modified CFPM2 to remove this numerical problem. Furthermore, we enhanced CFPM2 by incorporating a more general form of the nonlinear flow equation, where the flow exponent *m* can be user-defined. The intention of this methods note is to describe the functioning of the existing CFPM2 as well as the modified CFPM2. Furthermore, modifications on the source code were successfully validated by a test problem.

Computation of nonlinear flow with MODFLOW

Existing CFP Mode 2

Functionality of the existing CFPM2 is documented by Shoemaker et al. (2008a, 2008b), and Kuniansky et al. (2008). In summary, CFPM2's computation of laminar or turbulent flow is based on the dimensionless Reynolds number

$$Re = \frac{Vd}{\nu} \quad (2)$$

where V is the specific velocity or mean velocity [LT^{-1}], d is the mean void diameter [L], and ν is the kinematic viscosity of water [L^2T^{-1}]. In CFPM2 flow is considered to be turbulent if the Reynolds number is greater than the user-specified critical Reynolds numbers.

During operation, the CFPM2 algorithm converts the critical Reynolds number (Re_C) into a critical head difference (Δh_{crit}) (Shoemaker et al. 2008a) from:

$$\Delta h_{crit} = \frac{Re_C \nu \Delta L}{K_{lam} d} \quad (3)$$

where ΔL represents the length over which the head difference is measured [L], and K_{lam} is the laminar hydraulic conductivity [LT^{-1}]. Laminar flow is substituted by turbulent flow when the critical head difference is exceeded. Based on an approach for simulating turbulent flow in the vicinity of a wellbore (Halford 2000), a dimensionless adjustment factor F_{adj} is used to relate the laminar hydraulic conductivity (Shoemaker et al. 2008a; Kuniansky et al. 2008) with turbulent hydraulic conductivity K_{turb} [LT^{-1}] by using:

$$K_{turb} = F_{adj} K_{lam} \qquad (4)$$

The adjustment factor in CFPM2 is for media that goes turbulent at low Reynolds numbers as opposed to the adjustment used for pipes in Halford (2000). In summary, the adjustment factor in CFPM2 is:

$$F_{adj} = \sqrt{\frac{Re_C}{Re}} = \sqrt{\frac{K_{lam}\Delta h_{crit}}{K_{turb}\Delta h}} \qquad (5)$$

when $\Delta h > \Delta h_{crit}$ and $F_{adj} = 1$ when $\Delta h \le \Delta h_{crit}$. This approach was found to be well suited for describing turbulent flow observed in permeameter tests at low Reynolds numbers (Kuniansky et al. 2008).

Within the existing CFPM2, K_{turb} is determined every computational step. However, this iterative process (note Equations 4 and 5) is not controlled by an additional convergence criterion leading to an imperfect result for the adjustment factor while the convergence criterion for the matrix hydraulic heads is still fulfilled. Several computational steps are necessary to obtain the intended value for turbulent flow, resulting in a time step dependency even for steady state simulations (cf. Figure 2). If K_{turb} converged, and thus, is stable, CFPM2 computes flow according to the general power law (Equation 1) with an exponent m of 1.5 (cf. Figure 2).

Modification of CFP Mode 2

Modifications were made to (1) remove the dependency of turbulent flow on the number of time steps, (2) determine turbulent flow according to the generalized power law with a user-defined flow exponent m (Equation 1), and (3) account for the step-wise discharge behavior while transitioning from laminar to turbulent flow because laminar flow tends to stay laminar (Shoemaker et al. 2008a). This process is potentially important for conduit type flow but not observed in porous media and, therefore, conceptually not intended for CFPM2 (Shoemaker et al. 2008a).

To consider the step-wise discharge behavior, an upper critical Reynolds number Re_{C1} defines the transition from laminar to turbulent flow and a lower critical Reynolds number Re_{C2} describes transition from turbulent to laminar flow (cf. Kanda and Yanagiya 2008). Based on the two Reynolds numbers the corresponding critical heads Δh_{critC1} and Δh_{critC2} are computed according to Equation 3. In the case where laminar flow is transitioning to turbulent flow, the hydraulic conductivity is adjusted, if Δh exceeds Δh_{critC1}. Conversely, when turbulent flow is transitioning to laminar flow, the hydraulic conductivity is adjusted until Δh falls below Δh_{critC2}. If the step-wise discharge behavior conceptually is not intended both critical Reynolds numbers should be set to similar values.

The computation algorithm of the adjustment factor F_{adj} was modified such that laminar Darcian flow equals turbulent flow at some intersection point, which is defined by the lower critical Reynolds number Re_{C2} and a critical gradient I_{C2}. Therefore the following equation can be introduced:

$$K_{lam} I_{C2} = I_{C2}^{\frac{1}{m}} \beta^{-\frac{1}{m}} \qquad (6)$$

With this, $\beta^{1/m}$ is explicitly given as

$$\beta^{-\frac{1}{m}} = K_{lam} I_{C2}^{\frac{m-1}{m}} \qquad (7)$$

The commonly known Darcy equation with the formulation of K_{turb} (Equation 4) can be combined with the general power law (Equation 1 neglecting the linear term) yielding:

$$F_{adj} K_{lam} = I^{\frac{1-m}{m}} \beta^{-\frac{1}{m}} \qquad (8)$$

Substitute Equation 7 into Equation 8:

$$F_{adj} K_{lam} = I^{\frac{1-m}{m}} K_{lam} I_{C2}^{\frac{m-1}{m}} \qquad (9)$$

Finally, the adjustment factor F_{adj} can be directly determined as:

$$F_{adj} = \left(\frac{I}{I_{C2}}\right)^{\frac{1-m}{m}} \qquad (10)$$

Note this formulation allows the application of a user-defined flow exponent *m*. For instance, to compute conduit type flow the flow exponent is set to 2.0, which creates discharge equal to the Manning equation or the Colebrook-White formula.

The program listing of CFPM2 was slightly changed in order to consider the modified computation of the adjustment factor as well as the step-wise discharge behavior (Figure 1). As a first step, hydraulic heads are pre-calculated by MODFLOW-2005 based on the laminar hydraulic conductivity K_{lam}. After initial convergence, the computational loop is repeated with the modified CFPM2 algorithm to compute turbulent hydraulic conductivity K_{turb} based on Δh_{crit}, if necessary.

Figure 1 near here

Validation example

The validation test is designed to demonstrate the performance and accuracy of the nonlinear flow equations. Groundwater flow was focused to a 50 m long highly conductive structure to mimic a karst conduit. The discharge area is set to 0.785 m^2, which equals a conduit diameter of 1 m. By use of fixed-head boundary conditions on the inlet and outlet, a constant user-defined hydraulic gradient was established. For this scenario, the hydraulic gradient was set to 5×10^{-8}, which was sufficiently large to obtain turbulent flow (*Re* ~ 3,750). A steady state computation was accomplished with 100 equal time steps. The resulting discharge was computed with (a) the existing CFPM2, (b) the modified CFPM2 with different flow exponents *m*, and (c) the hybrid model CFP Mode 1, which computed turbulent flow according to the Colebrook-White equation (Shoemaker et al. 2008a). In addition, discharge was calculated directly with the Colebrook-White-, the Manning-, and the Darcy equation. Additional parameters of the test setup are given in Table 1.

Table 1 near here

Scenario A) Steady-state flow with constant hydraulic gradient

Figure 2 near here

As illustrated in Figure 2, the modified CFPM2 computes discharge correctly according to the underlying flow equations. With a flow exponent of $m = 1.5$ results of the modified CFPM2 are similar to the existing CFPM2 without the time step dependency. Using $m = 2.0$, the modified CFPM2 computes discharge according to the Manning equation. For comparison, the existing hybrid model CFP Mode 1 calculates discharge according to the Colebrook-White equation. In the transition regime where flow is not fully turbulent the discharge resulting from the Colebrook-White equation is slightly lower than that resulting from the Manning equation and CFPM2 with $m = 2.0$. For practical purposes the difference appears to be negligible though.

Scenario B) Transient flow with varying hydraulic gradient

Scenario B) verifies the changeover from laminar to turbulent conditions and vice versa. A transient model with eight stress periods was designed. Every period is computed with 100 time steps at 1 second each. The hydraulic gradient varies gradually from (a) clearly laminar conditions ($I_{Period1}$ = 2 x 10^{-9}) to (b) transitional conditions ($I_{Period2}$ = 5 x 10^{-9}, $I_{Period3}$ = 7 x 10^{-9}) to (c) turbulent conditions ($I_{Period4}$ = 2 x 10^{-8}, $I_{Period5}$ = 1 x 10^{-7}, $I_{Period6}$ = 4 x 10^{-8}) and (d) vice versa ($I_{Period7}$ = 6 x 10^{-9}, $I_{Period8}$ = 3 x 10^{-9}).

Figure 3 near here

Results demonstrate the correct functioning of the step-wise discharge behavior within the modified CFPM2 (Figure 3). Laminar discharge (Period 1 to 3) computed with the modified CFPM2 equals the Darcy equation. After Re_{C1} is exceeded, discharge is computed with the generalized power law (Equation 1) according to the user defined flow exponent (Period 4 to 6). During flow transitions from turbulent to laminar, discharge computed with the modified CFPM2 remains turbulent (Period 7) until the Reynolds number is less than Re_{C2} (Period 8).

Conclusions

Modifications were made to the turbulent flow approximation within CFPM2 of MODFLOW-2005 to remove a dependence of turbulent flow on the number of time steps. Furthermore, a more general turbulent flow formulation was incorporated with a user-defined exponent m that can increase or decrease the non-linearity between specific discharge and hydraulic gradient for correct simulation of turbulent flow in porous media or pipes. With an adequately selected flow exponent m, the modified version of CFPM2 mimics the existing version ($m = 1.5$) or a hybrid model with conduit flow in discrete pipes ($m = 2.0$).

The modified CFPM2 offers several advantages. Specifically, the new approximation is user friendly as parameter demand is limited to water temperature, conduit diameter and critical Reynolds numbers. Existing groundwater flow and constituent transport models can be easily recomputed with the modified CFPM2. In contrast to hybrid models, the laminar-turbulent continuum approach offers significant numerical advantages such as omission of additional iteration loops for coupling with a pipe-network.

On the other hand, there are limitations associated with the use of the modified CFPM2. For instance, it is necessary that cell discretization adequately reflects the conduit discharge area, or the water balance might be affected by discharge computed based on incorrect cross-sectional flow areas. Furthermore, CFPM2 parameters are uniformly valid in the whole layer meaning that all conduits have similar characteristics. Further work is necessary to improve the new algorithm, including efforts to reduce computer run times, increase compatibility with other MODFLOW processes and packages, remove the necessity of the linear precalculation (cf. Figure 1) to increase numerical stability, and incorporate natural heterogeneity in turbulent flow model parameters such as mean void diameters and critical Reynolds numbers. Removing these limitations potentially creates a straightforward and versatile continuum model, which considers nonlinear flow and therefore is vitally important for karst (and non-karst) aquifer modeling.

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Sadly, we have to report that our colleague and friend Dr. Christoph Rehrl died on 21 March 2010 at the age of 37 in a massive avalanche encountered during alpine ski touring.

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Figure captions

Figure 1: Cutaway from the MODFLOW-2005 CFP program flow chart (Shoemaker et al. 2008a, p. 16); the existing CFPM2 and modified CFPM2 processes are shown side by side.

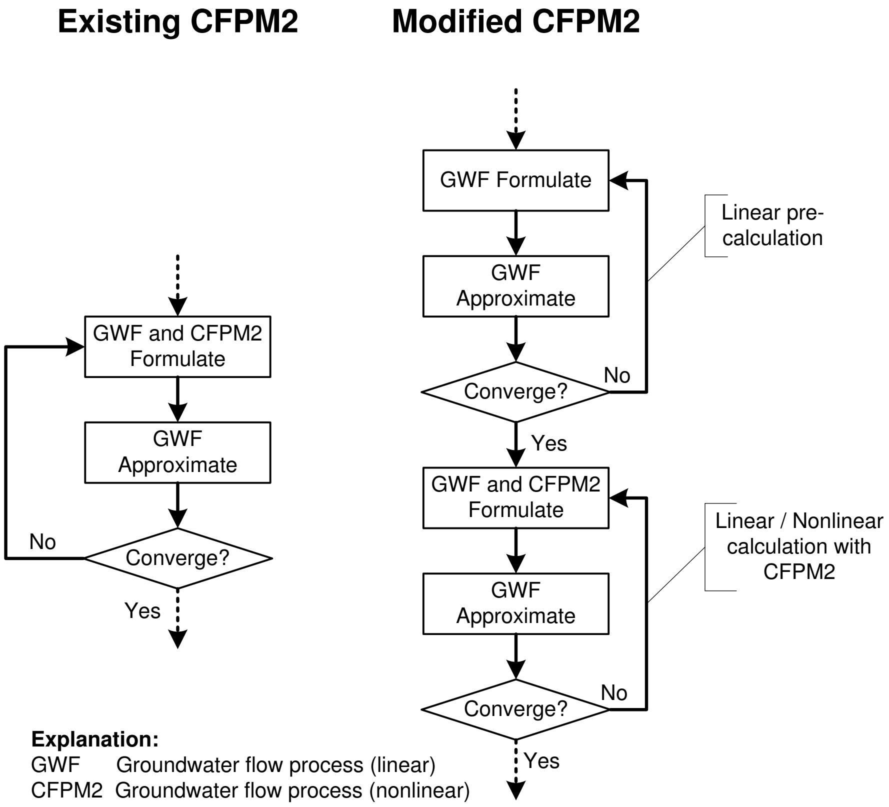
Figure 2: Dependency of computed discharge on the number of time steps in a steady-state model (Scenario A: turbulent flow with a hydraulic gradient of 5×10^{-8} in a single pipe)

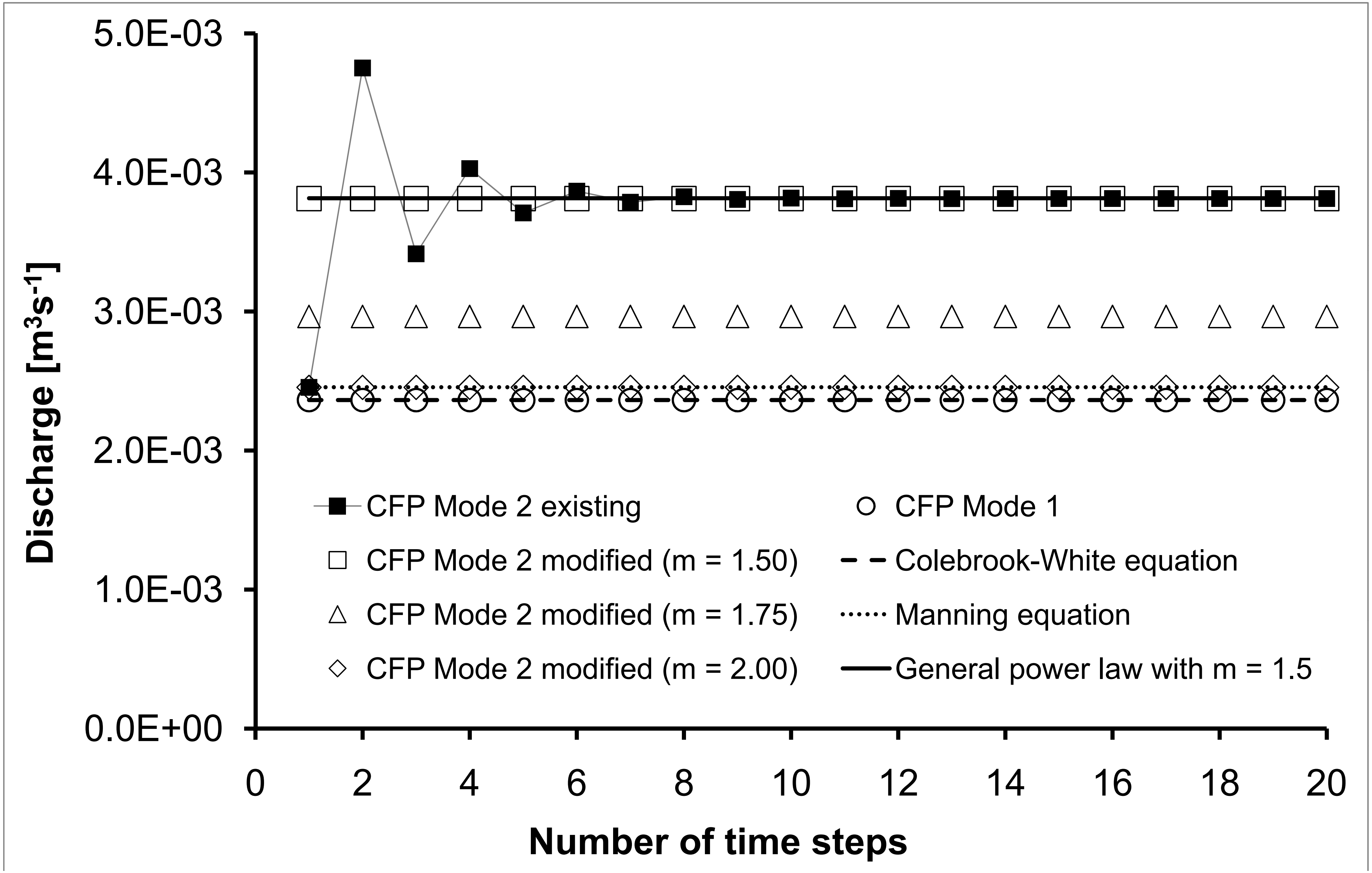
Figure 3: Computed discharge for Scenario B (transition from laminar flow to turbulent flow and vice versa) – transient model with eight stress periods (P1 to P8); discharge displayed was obtained after steady-state conditions were achieved

Tables

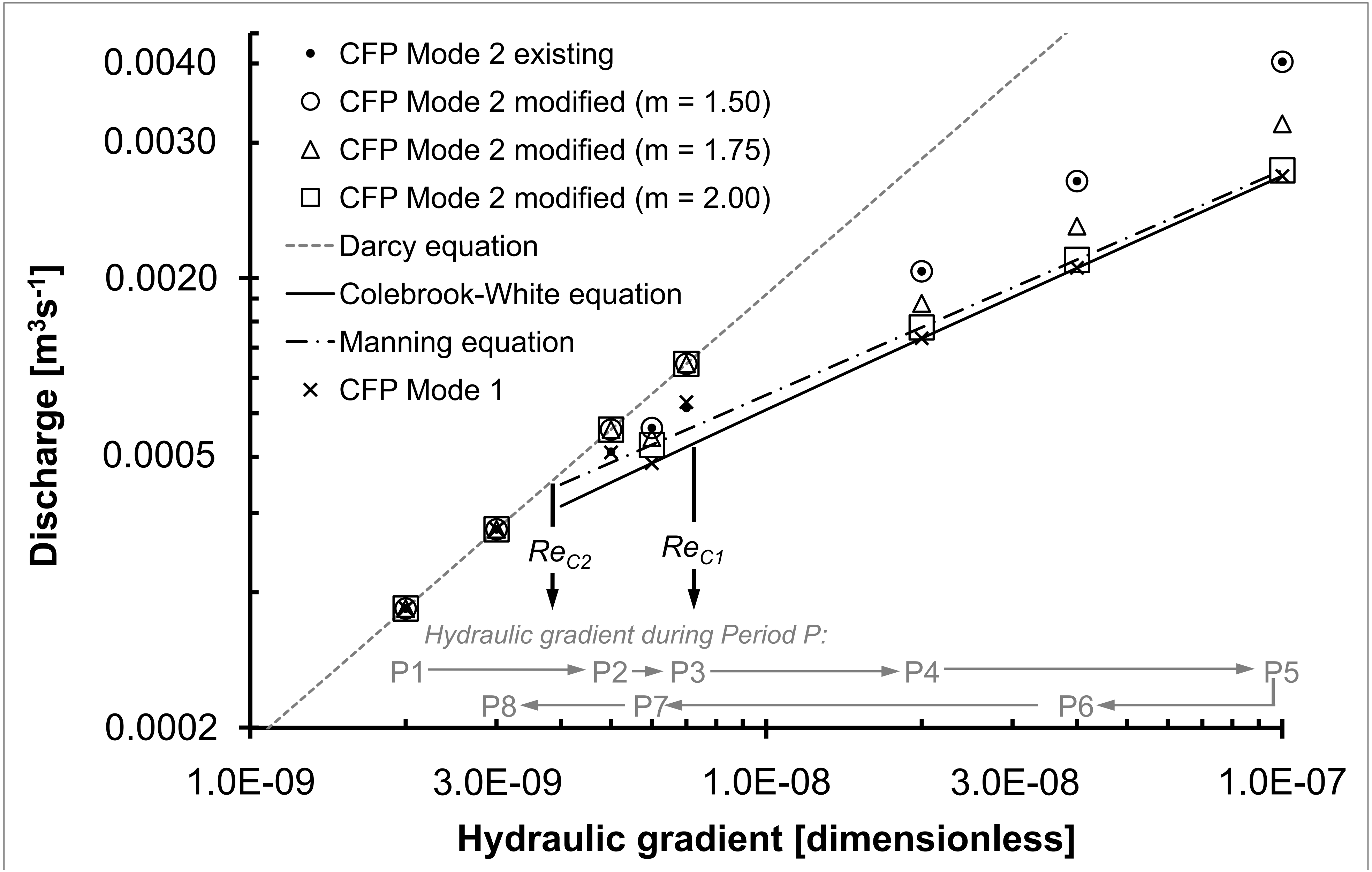
Table 1: Parameters of test setup

General parameter	
Upper critical Reynolds number	Re_{C1} = 1,275.2 (Re_{C1} = 637.7 for the existing CFPM2 because the step-wise behavior of discharge is conceptually not considered there)
Lower critical Reynolds number	Re_{C2} = 637.6
Time discretization	Scenario A): Steady state with 100 time steps each period Scenario B): Transient with 100 time steps a 1 second each period
Specific parameters for the continuum model	
Spatial discretization	5 cells with Δx = 10 m and $\Delta y = \Delta z$ = 0.886 m
Hydraulic conductivity	234,241.2 ms^{-1}
Hybrid model specific parameter	
Spatial discretization	5 nodes / 4 tubes with Δx = 10 m and pipe diameter = 1 m
Transfer to matrix	0
Pipe roughness	0.1 m


Existing CFPM2
Modified CFPM2
GWF Formulate
GWF Approximate
Converge?
No
Yes
Linear pre-calculation
GWF and CFPM2 Formulate
GWF Approximate
Converge?
No
Yes
Linear / Nonlinear calculation with CFPM2
GWF and CFPM2 Formulate
GWF Approximate
No
Converge?
Yes
Explanation:
GWF Groundwater flow process (linear)
CFPM2 Groundwater flow process (nonlinear)



5.0E-03
4.0E-03
3.0E-03
2.0E-03
1.0E-03
0.0E+00
Discharge [m3s-1]
0
2
4
6
8
10
12
14
16
18
20
Number of time steps
CFP Mode 2 existing
CFP Mode 2 modified (m = 1.50)
CFP Mode 2 modified (m = 1.75)
CFP Mode 2 modified (m = 2.00)
CFP Mode 1
Colebrook-White equation
Manning equation
General power law with m = 1.5



CFP Mode 2 existing
CFP Mode 2 modified (m = 1.50)
CFP Mode 2 modified (m = 1.75)
CFP Mode 2 modified (m = 2.00)
Darcy equation
Colebrook-White equation
Manning equation
CFP Mode 1
Discharge [m3s-1]
0.0040
0.0030
0.0020
0.0005
0.0002
Re_{C2}
Re_{C1}
Hydraulic gradient during Period P:
P1
P2
P3
P4
P5
P6
P7
P8
1.0E-09
3.0E-09
1.0E-08
3.0E-08
1.0E-07
Hydraulic gradient [dimensionless]