Appendix A. Capillary time step criterion

In this section, we identify the cause of the numerical instabilities that explicit methods suffer from at low flow rates when the capillary time step criterion (23) is not obeyed. We also derive this criterion. The contents of this section are not intended to constitute a formal proof of the stability of the presented time integration methods. The results derived herein are based on a linearized approximation of the pore network model. Although the application of results from a linearized analysis to general cases is somewhat simplistic, it is useful for highlighting key difficulties, see e.g. [26] pp. 347., and for deriving results that can be found to work in practice. For evidence of the actual stability of the time integration methods, it is therefore referred to the numerical tests performed in Section 9.

Consider a single link ij in a network and assume that p_i and p_j are given. Then the ODE (6) for the interface positions in the link is

$$\frac{\mathrm{d}\mathbf{z}_{ij}}{\mathrm{d}t} = \frac{q_{ij}\left(\mathbf{z}_{ij}\right)}{a_{ij}}. \tag{A.1}$$

We further assume that the flow rate in this link is low. This means that the node and capillary pressures almost balance at the current interface positions $\mathbf{z}^*_{ij}$, and thus $q_{ij}\left(\mathbf{z}^*_{ij}\right) \approx 0$. Also, we neglect the dependence of g_{ij} on the interface positions. Now rewrite (A.1) in terms $\Delta\mathbf{z}_{ij} = \mathbf{z}_{ij} - \mathbf{z}^*_{ij}$ and linearize the right hand side around $\mathbf{z}^*_{ij}$ to get

$$\frac{\mathrm{d}}{\mathrm{d}t}\Delta\mathbf{z}_{ij} \approx \frac{q_{ij}\left(\mathbf{z}^*_{ij}\right)}{a_{ij}} + \frac{g_{ij}\left(\mathbf{z}^*_{ij}\right)}{a_{ij}}\left(\sum_{z\in\mathbf{z}^*_{ij}} \frac{\partial c_{ij}}{\partial z}\right)\Delta\mathbf{z}_{ij}, \tag{A.2}$$

$$\approx \frac{g_{ij}\left(\mathbf{z}^*_{ij}\right)}{a_{ij}}\left(\sum_{z\in\mathbf{z}^*_{ij}} \frac{\partial c_{ij}}{\partial z}\right)\Delta\mathbf{z}_{ij}, \tag{A.3}$$

$$= \lambda\Delta\mathbf{z}_{ij}. \tag{A.4}$$

We can now read off the approximate ODE eigenvalue as

$$\lambda = \frac{g_{ij}\left(\mathbf{z}^*_{ij}\right)}{a_{ij}}\left(\sum_{z\in\mathbf{z}^*_{ij}} \frac{\partial c_{ij}}{\partial z}\right). \tag{A.5}$$

Without loss of generality, we may assume that $\lambda < 0$. If this is not the case, we interchange the indices i and j and redefine our spatial coordinate so that $z \to -z$ to get an ODE with negative λ. We therefore write the eigenvalue as

$$\lambda = -\frac{g_{ij}\left(\mathbf{z}^*_{ij}\right)}{a_{ij}}\left|\sum_{z\in\mathbf{z}^*_{ij}} \frac{\partial c_{ij}}{\partial z}\right|. \tag{A.6}$$

If the forward Euler method is to be stable on the linearized ODE, $\lambda\Delta t$ must lie in the stability region of the forward Euler method [26],

$$-2 < \lambda\Delta t < 0. \tag{A.7}$$

This is satisfied if we choose the time step such that

$$\Delta t < \frac{2a_{ij}}{g_{ij}\left(\mathbf{z}_{ij}^*\right)\left|\sum_{z\in\mathbf{z}_{ij}^*}\frac{\partial c_{ij}}{\partial z}\right|}. \tag{A.8}$$

The criterion (23) is obtained by demanding that (A.8) be satisfied for all links in the network. If the advective criterion (22) is used by itself and the link flow rates are low, then (A.8) is not necessarily satisfied for all links and we must expect numerical instabilities from the forward Euler method.

As the midpoint method has the same real-space stability region as the forward Euler method (A.7), the above reasoning and the criterion (23) can be applied for the midpoint method also.

The backward Euler method, on the other hand, is stable if [26]

$$\lambda\Delta t < 0, \tag{A.9}$$

and, because λ is negative, it is stable with any positive Δt for this linearized problem.

Appendix B. Jacobian matrix for the semi-implicit method

In order to solve (35) using the numerical method described in Section 7, it is necessary to have the Jacobian matrix of $\mathbf{F}$. This matrix may be written as

$$\frac{\partial F_i}{\partial p_j^{(n+1)}} = \delta_{ij}\sum_k \frac{\partial q_{ik}^{(n+1)}}{\partial p_i^{(n+1)}} + \left\{1-\delta_{ij}\right\}\frac{\partial q_{ij}^{(n+1)}}{\partial p_j^{(n+1)}}. \tag{B.1}$$

The derivative of $q_{ik}^{(n+1)}$ with respect to $p_i^{(n+1)}$ can be found by differentiation of (32) with respect to $p_i^{(n+1)}$ and application of the chain rule,

$$\frac{\partial q_{ij}^{(n+1)}}{\partial p_i^{(n+1)}} = -g_{ij}^{(n)} + g_{ij}^{(n)}\frac{\partial c_{ij}^{(n+1)}}{\partial p_i^{(n+1)}}, \tag{B.2}$$

$$= -g_{ij}^{(n)} + g_{ij}^{(n)}\frac{\mathrm{d}c_{ij}^{(n+1)}}{\mathrm{d}q_{ij}^{(n+1)}}\frac{\partial q_{ij}^{(n+1)}}{\partial p_i^{(n+1)}}. \tag{B.3}$$

This can be solved for the desired derivative to yield

$$\frac{\partial q_{ij}^{(n+1)}}{\partial p_i^{(n+1)}} = -\frac{g_{ij}^{(n)}}{1-g_{ij}^{(n)}\frac{\mathrm{d}c_{ij}^{(n+1)}}{\mathrm{d}q_{ij}^{(n+1)}}}. \tag{B.4}$$

Herein, the derivative of capillary pressure with respect to flow rate is

$$\frac{\mathrm{d}c_{ij}^{(n+1)}}{\mathrm{d}q_{ij}^{(n+1)}} = \frac{2\sigma_{\mathrm{wn}}}{r_{ij}}\sum_{z\in\mathbf{z}_{ij}^{(n+1)}}(\pm 1)\sin\left(2\pi\chi_{ij}(z)\right)\frac{\mathrm{d}\chi_{ij}}{\mathrm{d}z}\frac{2\pi\Delta t^{(n)}}{a_{ij}}, \tag{B.5}$$

for the specific choice of capillary pressure model given by (9).

As the pore network model is linear in the node pressures, it is intuitive that the effect on the link flow rate of increasing the pressure in the node at one end of a link is the same as decreasing it, by the same amount, in the node at the other end. Thus we may write

$$\frac{\partial q_{ij}^{(n+1)}}{\partial p_j^{(n+1)}} = -\frac{\partial q_{ij}^{(n+1)}}{\partial p_i^{(n+1)}}. \tag{B.6}$$

This equation may be more formally derived by differentiating (32) with respect to $p_j^{(n+1)}$ to get

$$\frac{\partial q_{ij}^{(n+1)}}{\partial p_j^{(n+1)}} = g_{ij}^{(n)} + g_{ij}^{(n)} \frac{\partial c_{ij}^{(n+1)}}{\partial p_j^{(n+1)}}, \tag{B.7}$$

$$= g_{ij}^{(n)} + g_{ij}^{(n)} \frac{\mathrm{d}c_{ij}^{(n+1)}}{\mathrm{d}q_{ij}^{(n+1)}} \frac{\partial q_{ij}^{(n+1)}}{\partial p_j^{(n+1)}}, \tag{B.8}$$

and, solving for the desired derivative,

$$\frac{\partial q_{ij}^{(n+1)}}{\partial p_j^{(n+1)}} = \frac{g_{ij}^{(n)}}{1 - g_{ij}^{(n)} \frac{\mathrm{d}c_{ij}^{(n+1)}}{\mathrm{d}q_{ij}^{(n+1)}}}. \tag{B.9}$$

Comparison of (B.4) and (B.9) gives the intuitive result (B.6).

The addition of F_m (40) to the non-linear system for the specified flow rate boundary condition, introduces some new terms in the Jacobian matrix of $\mathbf{F}$. The derivatives of F_m with respect to the node pressures are

$$\frac{\partial F_m}{\partial p_k^{(n+1)}} = \sum_{ij\in\Omega} \left\{ \delta_{ki} \frac{\partial q_{kj}^{(n+1)}}{\partial p_k^{(n+1)}} + \delta_{kj} \frac{\partial q_{ik}^{(n+1)}}{\partial p_k^{(n+1)}} \right\}, \tag{B.10}$$

where link flow rate derivatives are calculated using (B.4) and (B.6) and the derivative with respect to ΔP is

$$\frac{\partial F_m}{\partial (\Delta P)} = -\sum_{ij\in\Omega} \frac{g_{ij}^{(n)}}{1 - g_{ij}^{(n)} \frac{\mathrm{d}c_{ij}^{(n+1)}}{\mathrm{d}q_{ij}^{(n+1)}}}. \tag{B.11}$$

The additional terms corresponding to the derivatives with respect to ΔP of the mass balance equations for each node k with unknown pressures are

$$\frac{\partial F_k}{\partial (\Delta P)} = \sum_{ij\in\Omega} \left\{ \delta_{kj} - \delta_{ki} \right\} \frac{g_{ij}^{(n)}}{1 - g_{ij}^{(n)} \frac{\mathrm{d}c_{ij}^{(n+1)}}{\mathrm{d}q_{ij}^{(n+1)}}}. \tag{B.12}$$