Grid refinement for modeling multiphase flow in discretely fractured porous media

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Received 1 April 1998; received in revised form 1 February 1999

Abstract

A study of the effects of grid discretization on the migration of DNAPL within a discrete-fracture network embedded in a porous rock matrix is presented. It is shown that an insufficiently fine discretization of the fracture elements can lead to an overprediction of the volume of DNAPL that continues to migrate vertically at the intersection of a vertical and horizontal fracture. Uniform discretization of elements at the scale of one centimetre (or less) accurately resolved the density and capillary pressure components of the head gradient in the DNAPL. An alternative, non-uniform method of discretization of elements within the discrete-fracture network is presented whereby only fracture elements immediately adjacent to fracture intersections are refined. To further limit the number of elements employed, the porous matrix elements adjacent to the fracture elements are not similarly refined. Results show this alternative method of discretization reduces the numerical error to an acceptable level, while allowing the simulation of field-scale DNAPL contamination problems. The results from two field-scale simulations of a DNAPL-contaminated carbonate bedrock site in Ontario, Canada are presented. These simulations compare different methods of grid discretization, and highlight the importance of grid refinement when simulating DNAPL migration problems in fractured porous media. © 1999 Published by Elsevier Science Ltd. All rights reserved.

Keywords: Modeling; Multiphase flow; Fractured porous media; Grid refinement

1. Introduction

Problems of groundwater contamination by hazardous non-aqueous phase liquids (NAPLs) are of great concern throughout the industrialized world. Numerical models capable of simulating multiphase flow and phase partitioning processes have been created in an effort to help understand the behavior and fate of NAPLs in the subsurface. If the geologic strata in question contain units of low primary permeability but significant secondary permeability due to the presence of a network of interconnected fractures within the material, the task of modeling the system becomes more complicated. It is necessary in this case to recognize the possibility of rapid transport of the NAPL within the fracture network, while also incorporating the effect that the surrounding matrix can have on NAPL migration within the fracture network.

Laboratory studies [4] and mathematical modeling [5] have shown that the diffusion of dissolved contaminants from the fracture network to the surrounding rock matrix causes the eventual disappearance of the NAPL from the fracture network. Ref. [9] showed that in addition to causing the eventual disappearance of NAPL from a fracture embedded in a porous matrix, matrix diffusion could retard the migration of an NAPL front within a single vertical fracture. This numerical modeling study used the numerical model CompFlow that simulated, in three-dimensions, multiphase flow within a discrete-fracture network embedded in a porous matrix, including representation of phase partitioning and aqueous-phase transport processes in the fractures and in the porous matrix.

Previous studies have shown that for the simulation of multiphase flow in porous media, the use of an insufficiently fine discretization can result in reduced NAPL mobility [7]. However, little work has been attempted concerning the effects of discretization when
simulating NAPL migration within a fractured porous medium. The purpose of this study is to use the numerical model CompFlow to investigate how the discretization of discrete-fracture elements embedded within a porous media may be optimized for the accurate simulation of NAPL contamination problems.

2. Numerical model CompFlow

The CompFlow model uses a finite-volume discretization in which the rock matrix is represented by three-dimensional block elements, while the discrete-fracture elements are represented by two-dimensional planar, rectangular elements. The advective and diffusive fluxes of each component in each fluid phase are calculated at each time step, based on the values of the primary variables in the adjacent fracture and rock matrix elements. A schematic diagram of this coupling is shown in Fig. 1.

The capillary pressure versus saturation relationship within a rough-walled fracture has been shown to be adequately represented by a Brooks–Corey type functional relationship [8]. Capillary pressure curves used in this study are based on the work of [3], and further details of their incorporation into the numerical model may be found in Ref. [9]. Fig. 2(a) shows the capillary pressure curves for a rough-walled fracture with an equivalent hydraulic aperture of 200 \( \mu \)m, and another with an equivalent hydraulic aperture of 100 \( \mu \)m. The value of the capillary pressure shown at a water saturation equal to unity will be referred to as the “entry pressure” of the fracture, and represents the minimum pressure required for the non-aqueous phase to enter a water saturated fracture. Note that the entry pressure of a rough-walled fracture with an effective hydraulic aperture of 200 \( \mu \)m will be less than that of an idealized 200-\( \mu \)m smooth-walled fracture.

3. DNAPL migration in a fracture network

3.1. Theory

Fig. 3 shows a conventional finite volume discretization of a vertical fracture meeting a horizontal fracture. For simplicity, consider the case of single phase flow. Let

\[
\psi_i = P_i + \rho g z_i, \tag{1}
\]

where \( P_i \) is the fluid pressure, \( \rho \) is the fluid density, \( g \) is the gravitational acceleration constant, and \( z_i \) is the
This will cause some difficulty in simulating multiphase flow problems, because the timestep will be reduced when the DNAPL invades the junction cell. Consequently, it is desirable to eliminate node $o$ from the discrete equations.

Consider a finite volume discretization of the steady-state single phase pressure equation at node $o$

$$\sum_{j \in \gamma_{jo}} \frac{\gamma_{jo}}{\mu} (\psi_j - \psi_o) = 0, \quad (2)$$

where

$$\gamma_{jo} = A_{jo} k_{jo} \Delta x_{jo},$$

where $A_{jo}$ the interfacial area between cell $j$ and cell $o$, $k_{jo}$ the absolute permeability, $\mu$ the viscosity, $A_{jo}$ the distance between $j$ and node $o$,

$$\gamma_{\odot} = \{i, j, k, m\}, \quad (3)$$

where $\gamma_{\odot}$ is the set of neighbours of node $o$. Eq. (2) then implies that

$$\psi_o = \frac{\sum_{j \in \gamma_{\odot}} \gamma_{jo} \psi_j}{\sum_{j \in \gamma_{\odot}} \gamma_{jo}}. \quad (4)$$

Now, consider flow into cell $i$ from cell $o$, $F_{oi}$

$$F_{oi} = \frac{\gamma_{io}}{\mu} (\psi_o - \psi_i). \quad (5)$$

Using Eq. (4) in Eq. (5) gives an expression directly coupling flow into cell $i$ in terms of nodal values in cells $j, k, m$

$$F_{oi} = \sum_{j \in \gamma_{io}} F_{ji},$$

$$F_{ji} = \frac{\gamma_{ji}}{\mu} (\psi_j - \psi_i),$$

$$\gamma_{ji} = \frac{\gamma_{io} \gamma_{jo}}{\sum_{j \in \gamma_{\odot}} \gamma_{jo}}. \quad (6)$$

In other words, the flow from cell $j$ into cell $i$ can be computed directly as

$$F_{ji} = \frac{\gamma_{ji}}{\mu} (\psi_j - \psi_i). \quad (7)$$

Eq. (7) can be generalized to the multiphase case. For example, if flow of a non-aqueous phase $N$ between node $i$ and node $j$ is desired, then this is

$$F_{ji}^N = (k_i^N)_{ji}^{1/2} \frac{\gamma_{ji} (\psi_j^N - \psi_i^N)}{\mu^N}, \quad (8)$$

where $(k_i^N)_{ji}^{1/2}$ the interface value of relative permeability of NAPL phase,

$$\psi_j^N = \rho_j^N g z_j,$$

where the relative permeability term is upstream weighted.

Consider a DNAPL entering the junction in Fig. 3 from node $i$. If we assume that the ambient groundwater flow is from left to right, then the DNAPL can either flow initially from node $i$ to node $k$, or from node $i$ to node $m$. The actual path will be determined by the magnitude of two competing forces: gravitational and capillary. The discrete flow of DNAPL between node $i$ and node $k$ due to capillary forces will be proportional to

Capillary flow $\propto P_i^c - P_k^c$, \quad (9)

where $P_i^c$ is the capillary pressure at node $i$. The discrete flow due to gravitational forces is proportional to

Gravity flow $\propto \Delta \rho g (z_i - z_k)$, \quad (10)

where $\Delta \rho$ is the density difference between non-aqueous and aqueous phases.

Consequently, the path taken by a DNAPL migrating downwards from node $i$ will be determined by the relative aperture sizes of the fractures at nodes $k$ and $m$. For example, if the fracture at node $k$ has a hydraulic aperture of 200 $\mu$m, while the fracture at node $m$ has a hydraulic aperture of 100 $\mu$m, the DNAPL will initially enter fracture $k$ due to its lower entry pressure as shown in Fig. 2(a). As the relative saturation of DNAPL increases at node $k$, the capillary pressure will rise. If the capillary pressure at node $k$ reaches the value indicated by the dotted line in Fig. 2(a), then it is equal to the

![Fig. 3. Discretization of a vertical horizontal fracture junction.](image-url)
entry pressure at node \( m \). As the fracture element size (and hence spatial discretization error) approaches zero, this will be the point at which the DNAPL will enter the fracture at node \( m \), in this case at a relative DNAPL saturation of about 91%, as shown by the dotted lines in Fig. 2(a).

3.2. Comparison of results for several uniform refinements of fracture network

To investigate the effect of the numerical discretization on the DNAPL migration pathway in such a system, a simple 12 m \( \times \) 12 m domain of unit thickness was constructed. It consists of a single water-saturated vertical fracture intersecting a single horizontal fracture within a porous matrix block as shown in Fig. 4. The porosity and hydraulic conductivity of the rock matrix equal 0.03 and \( 8 \times 10^{-8} \) m/s, respectively. The vertical fracture has a hydraulic aperture of 100 \( \mu \)m and the horizontal fracture has a hydraulic aperture of 200 \( \mu \)m. The permeabilities of the fractures were assigned values according to their apertures using the conventional cubic law. The relative permeability curves for both fractures are provided in Fig. 2(b). The ambient hydraulic gradient is horizontal from left to right, with a value of 0.005. The DNAPL is composed of a single component with the physiochemical properties of a typical poly-chlorinated-biphenyl (PCB). The properties of the DNAPL are provided in Table 1. The DNAPL will be released at the top of the vertical fracture at a constant rate of 400 ml/day for a period of thirty days.

The fractures were discretized at five different levels of refinement: \( \Delta x = \Delta z = 200, 25, 5, 1 \) and 0.1 cm. To allow the problem to remain tractable, the discretization of the matrix elements was not refined beyond \( \Delta x = \Delta z = 25 \) cm, and fluid fluxes between the matrix and fracture elements were ignored.

The level of refinement of the fracture network had a significant effect on the migration pathway of the infiltrating DNAPL front. Fig. 5 shows the percentage of the total DNAPL flux arriving at the fracture intersection that entered the horizontal fracture as a function of time for the various levels of discretization. As the discretization was refined, the flux of DNAPL through the horizontal fracture increased, particularly at early time when the infiltrating DNAPL first reached the fracture intersection at a time of approximately two days. As discussed in Section 3.1, the DNAPL initially enters the large-aperture horizontal fracture exclusively, due to its lower entry pressure. However, the entry pressure of the narrow vertical fracture below the fracture intersection is overcome soon after, with approximately 15–20% of the steady-state flux of DNAPL that reaches the fracture intersection continuing downwards, depending on the level of discretization.

The sensitivity of the pathway taken by the infiltrating DNAPL to the mesh discretization is due to the spatial discretization error involved in calculating the gravity and capillary pressure gradients at the fracture intersection. The gravity gradient is uniform, and the calculated DNAPL flow due to gravitational forces increases as the vertical length of the fracture elements increases, as shown in Eq. (10). With reference to Fig. 3, the capillary pressure difference between the horizontal and vertical fracture is independent of the distance between cells \( i \) and \( k \), and the calculated capillary pressure gradient will decrease as the length of the fracture ele-

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Table 1

<table>
<thead>
<tr>
<th>Physiochemical property</th>
<th>PCB</th>
<th>Aqueous phase</th>
</tr>
</thead>
<tbody>
<tr>
<td>Free solution diffusion coefficient in water (m²/day)</td>
<td>( 8.7 \times 10^{-5} )</td>
<td>N/A</td>
</tr>
<tr>
<td>Interfacial tension of NAPL–Water system (N/m)</td>
<td>( 4.4 \times 10^{-2} )</td>
<td>N/A</td>
</tr>
<tr>
<td>Liquid compressibilities (kPa⁻¹)</td>
<td>( 3.0 \times 10^{-6} )</td>
<td>( 4.3 \times 10^{-7} )</td>
</tr>
<tr>
<td>Viscosities (kPa day)</td>
<td>( 4.63 \times 10^{-10} )</td>
<td>( 1.4 \times 10^{-11} )</td>
</tr>
<tr>
<td>Mass density (kg/m³)</td>
<td>1400</td>
<td>1000.1</td>
</tr>
<tr>
<td>Equilibrium mole fraction in aqueous phase</td>
<td>( 1.5 \times 10^{-8} )</td>
<td>N/A</td>
</tr>
<tr>
<td>Aqueous phase solubility (mg/l units)</td>
<td>0.25 mg/l</td>
<td>N/A</td>
</tr>
</tbody>
</table>
ments increases. A coarse discretization can result in an over-prediction of the volumetric flux of DNAPL that continues vertically downwards within the fracture, following the path $i \rightarrow m$ in Fig. 3.

The illustrative problem presented above indicates that for this scenario, a further grid refinement beyond $\Delta x = \Delta z = 1.0$ cm does not significantly decrease the numerical error in the solution. The point at which further refinement yields little improvement will be affected by the density difference between the DNAPL and water. With a relative density of 1.5 times that of water, the DNAPL used in these simulations is near the upper end of the range of densities of common DNAPL contaminants found in groundwater. Thus, the alternative non-uniform discretization scheme discussed hereafter is designed to produce the maximum level of refinement necessary near a fracture intersection, but without the need for a concomitantly high level of refinement in the adjacent rock matrix.

### 3.3. Alternative to uniform grid refinement in fracture network

In the previous example problem containing only two fractures, it was possible to discretize the entire fracture domain at the scale of one centimetre. However, when applying the numerical model to a typical field-scale DNAPL contamination problem, it is not possible to discretize the entire fracture network with this degree of grid refinement. Therefore, it is desirable to develop a refinement scheme that locally refines the grid adjacent to the fracture intersections, as it is in these locations that the numerical error resulting from the discrete approximation has the greatest effect on the solution.

By comparing various non-uniform discretization schemes to the solution obtained with the uniform 1.0 cm discretization, it was found that refining only the first two elements adjacent to the fracture intersection could eliminate much of the numerical error in the solution. Immediately above and below the horizontal fracture, $\Delta z$ was increased from 0.1 cm to 1 cm to 200 cm over the first three elements, while to the left and right of the vertical fracture, $\Delta x$ was increased in an identical fashion.

A comparison of the percentage of DNAPL flux entering the horizontal fracture in a simulation employing this method of non-uniform mesh refinement, and in a simulation using the uniform one centimetre discretization is given in Fig. 6. The general agreement between these two solutions indicates that the numerical error in the solution can be kept acceptably small by employing a refined grid adjacent to fracture intersections and a relatively coarse discretization in the remainder of the domain.

### 3.4. Alternative to complete refinement of the matrix elements

In traditional finite-element discretization schemes that make use of mixed element types to represent high conductivity features such as fractures or well bores, the nodes of the high conductivity elements are common to those of the adjacent matrix elements, making the calculation of fluxes between the two element types unnecessary [11,12]. This use of shared nodes between two different element types does not allow the possibility of refining the discretization within the fracture network.
while at the same time retaining a more coarse discretization within the rock matrix.

If the normal process of refining both the fracture and matrix elements is followed, the number of matrix elements increases rapidly. The alternative is to refine the discretization exclusively within the fracture network while leaving the discretization within the matrix cells unchanged. The difference in these two approaches is conceptualized in Fig. 7, which shows the proliferation of additional matrix elements if the mesh is refined using the traditional approach (Fig. 7(b)). This level of discretization within the matrix elements may not be necessary given the lower permeability and lower flow velocities within the matrix.

For the discretization scheme depicted in Fig. 7(c), in which the refinement takes place only within the fracture network, it is desirable to minimize the number of non-zero entries in the global stiffness matrix. This can be done by coupling only the largest fracture element with the adjacent matrix element, but calculating the flux between the matrix and fracture elements as though it takes place across the entire surface area of the matrix element. For example, in Fig. 7(c), the matrix node is connected only to a single fracture node in the horizontal direction, and a single node in the vertical direction. The smaller fracture elements adjacent to the fracture intersection are then only linked to their neighbouring fracture elements and not to the neighbouring matrix element. This is similar to the multiple interacting continua (MINC) concept introduced by [6]. This reduces the storage requirements and speeds processing without significantly affecting the solution. Fig. 8 compares results obtained using the alternative method of coupling the fracture and matrix elements, as depicted in Fig. 7(c), to those based on a conventional discretization in which every fracture element is coupled to a matrix element as depicted in Fig. 7(b).

4. Discretization effects in a field-scale DNAPL infiltration problem

We have demonstrated, using a simple example, that insufficient discretization of discrete-fracture elements near fracture intersections can result in significant numerical errors in the migration pathway taken by an infiltrating DNAPL front. Specifically, a coarse discretization employed at the intersection of a wide aperture horizontal fracture and narrower vertical fracture produces an overprediction of the vertical flux of DNAPL, and a corresponding underprediction of the volume of DNAPL that enters the horizontal fracture. This has important implications with regard to the prediction of the maximum horizontal and vertical extent that a DNAPL-contaminated zone could occupy in a fractured rock.

We have also presented an alternative discretization scheme that minimizes storage requirements and maximizes the numerical efficiency of the model, while also keeping the numerical error arising from the discrete approximation at an acceptably small level. This
The discretization scheme will now be applied to a field-scale problem to investigate the effect of this grid refinement technique on a DNAPL infiltration problem involving a complex network of fractures in a stratified carbonate bedrock.

The physical system for simulations that follow are based on the geological setting in the Niagara Peninsula where a former PCB waste transfer facility was located near the town of Smithville, Ontario. The simulation results are likely to be applicable to similar settings involving DNAPL migration in fractured carbonate rocks. The hydrostratigraphy of the Smithville site is shown in Fig. 9, and consists of approximately a 6 m thickness of clay till overburden containing a thin layer of sandy till at its base, which is in turn underlain by about 40 m of carbonate bedrock weathered to varying degrees. The Rochester shale constitutes the base of the system and it is treated here as an impermeable unit.

The network of fractures within the carbonate bedrock has been studied in great detail by physical examination of rock core retrieved from angled boreholes, and by hydraulic packer testing performed in these angled boreholes [2]. The results from these field investigations have been used as a guide in assigning parameters such as fracture spacing, fracture aperture range and fracture density to be used in the generation of a fracture network within the vertical cross section depicted in Fig. 9. The resulting fracture network is shown in Fig. 10, and the range from which fracture aperture values were randomly assigned for each hydrostratigraphic unit are given in Table 2. The relative permeability relationships within the fractures are invariant with fracture aperture and remain identical to those given in Fig. 2(b). The capillary pressure curves will retain the same shape as that given in Fig. 2(a), but will shift vertically because the entry pressure varies inversely with the fracture aperture.

The range in aperture values given for the clay overburden in Table 2, is based on field excavations performed at the Smithville site which have shown the till to be fissured throughout its entire thickness with predominantly vertical fractures and macropores [13]. Many of the fractures appear to be aligned with vertical fractures in the underlying bedrock. This has been incorporated into the model of the site by including several fractures, which are continuous through the overburden zone and extend into the uppermost zone of fractured bedrock. The porosity and permeability values assigned to the clay are typical of similar deposits studied in Southern Ontario. The relative permeability curves for the clay matrix are generated from a simple power function and the capillary pressure relationship is based on a compilation of data by El-Kadi [1].

The capillary pressure curves for each of the hydrostratigraphic units within the carbonate rock sequence are taken from data compiled by Stout [10]. Although the capillary pressure curves have yet to be measured for the rock core collected at the Smithville site, microscopic examination of thin sections of rock cores have yielded some insight into the apparent sizes of the pore throat diameters in each unit. Different capillary pressure curves were assigned to each of the hydrostratigraphic

Table 2
Matrix properties of geologic units at Smithville, Ontario site

<table>
<thead>
<tr>
<th>Geologic unit</th>
<th>( K_v ) (m/s)</th>
<th>( K_i ) (m/s)</th>
<th>Porosity</th>
<th>Fracture aperture range (( \mu m ))</th>
</tr>
</thead>
<tbody>
<tr>
<td>Overburden</td>
<td>( 8.0 \times 10^{-9} )</td>
<td>( 8.0 \times 10^{-9} )</td>
<td>0.5</td>
<td>200–1000</td>
</tr>
<tr>
<td>Sandy till</td>
<td>( 8.0 \times 10^{-5} )</td>
<td>( 8.0 \times 10^{-5} )</td>
<td>0.3</td>
<td>200–1000</td>
</tr>
<tr>
<td>Permeable dolostone</td>
<td>( 4.0 \times 10^{-8} )</td>
<td>( 8.0 \times 10^{-8} )</td>
<td>0.03</td>
<td>100–400</td>
</tr>
<tr>
<td>Weathered dolostone</td>
<td>( 8.0 \times 10^{-6} )</td>
<td>( 8.0 \times 10^{-6} )</td>
<td>0.15</td>
<td>100–400</td>
</tr>
<tr>
<td>Tight dolostone</td>
<td>( 8.0 \times 10^{-9} )</td>
<td>( 8.0 \times 10^{-9} )</td>
<td>0.03</td>
<td>50–200</td>
</tr>
</tbody>
</table>
units within the carbonate sequence based on this visual examination. The capillary pressure relationships and relative permeability curves for the dolostone rocks are provided in Fig. 11(a) and (b).

The 300 m long, 43 m thick, vertical model cross section is coincident with the regional direction of groundwater flow at the site. Recharge is applied across the upper boundary at a constant rate of five mm/year, while the bottom boundary is impermeable and taken to be the contact with the underlying Rochester shale. The boundary conditions along the left and right sides of the domain are constant head boundaries, defined such that the ambient groundwater flow is left to right through the domain under a hydraulic gradient of 0.005.

The single-component DNAPL assumed here has the physiochemical characteristics of a typical poly-chlorinated biphenyl as given in Table 1, although analyses of DNAPL taken from the site indicate that other components including TCE are present. The DNAPL is released at the ground surface for a period of one year from a pool approximately 30 m wide that intersects several fractures in the clay overburden as shown in Fig. 10. The DNAPL pool is assumed to have a constant depth of 0.30 m of PCB throughout the duration of the simulations.

Fig. 12 shows a comparison between simulated DNAPL saturations after a time equal to six months obtained with the fracture network shown in Fig. 10, but using the two different methods to discretize the fracture network. The simulation shown in Fig. 12(b) used a fracture mesh with elements adjacent to each fracture intersection refined as described earlier, while Fig. 12(a) used an identical discretization without the additional refinement adjacent to the fracture intersections.

By more accurately resolving the migration of DNAPL into the wide aperture horizontal fractures at the fracture intersections, the horizontal and vertical extent of the zone of DNAPL contamination within the bedrock extends changes dramatically. The increased tendency for horizontal spreading of the DNAPL when using the refined mesh results in a much shallower DNAPL plume that extends much further downgradient of the surficial release area than is the case when an inappropriately coarse mesh is used.
5. Conclusions

Field-scale simulation of the migration of DNAPL is a valuable approach in determining the extent of the spread of DNAPL in fractured rocks. Simulation of such sites is also a useful tool for evaluating alternative remediation scenarios.

If discrete fractures are modeled, then traditional discretization methods require a very large number of finite volume cells. Many of these cells have very small volumes, which cause difficulties for the convergence of the non-linear iteration required for modeling multiphase flow. As demonstrated in this article, use of a coarse discretization, especially near the intersection of a wide aperture horizontal fracture and a narrow vertical fracture, may produce completely misleading results.

Several methods are described for constructing a discretization, which produces acceptably accurate results, while minimizing storage and computational cost. These techniques were demonstrated in a field-scale problem based on a former PCB waste transfer site near Smithville Ontario. Use of a typical coarse grid on this problem resulted in a significant overprediction of the vertical extent of DNAPL penetration compared to the discretization method developed in this work. Consequently, use of an inappropriate discretization would have important ramifications for the design of a remediation process.

The discretization methods described in this article allowed simulation of complex multiphase flow at a fractured carbonate site on an inexpensive workstation. Traditional discretization methods would have required computing resources well beyond the budget for this project. We note that the adaptive mesh refinement methods developed in this work are a priori, based on our knowledge of the physical system. A challenging avenue for future research would be to develop a posteriori methods for simulating fractured systems. These techniques would automatically adjust the mesh based on an error estimator.

Acknowledgements

Funding for this work was provided by the Smithville Phase IV Bedrock Remediation Program, the Waterloo Centre for Groundwater Research (now CRESTech), the Information Technology Research Centre (now CITO), and grants to E.A. Sudicky and P.A. Forsyth by the Natural Sciences and Engineering Research Council of Canada (NSERC).

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