NUMERICAL MODELLING OF GRAIN-DISPLACING GAS HYDRATE MORPHOLOGIES

Gabrielle Wojtowitz*
School of Civil Engineering & the Environment
University of Southampton
Southampton, SO17 1BJ
UNITED KINGDOM

Antonis Zervos
School of Civil Engineering & the Environment
University of Southampton
Southampton, SO17 1BJ
UNITED KINGDOM

Chris R. I. Clayton
School of Civil Engineering & the Environment
University of Southampton
Southampton, SO17 1BJ
UNITED KINGDOM

ABSTRACT
The understanding of the effect of hydrate on marine host sediments is fundamental for the detection and quantification of gas hydrate from exploratory seismic survey data. For the interpretation of seismic data, effective medium models are used, which employ different theoretical assumptions to relate wave velocities to gas hydrate content of the sediment. Methane gas hydrates occur in situ in a variety of morphologies, generally classed as either pore-filling or grain-displacing. There are effective medium models for pore-filling morphologies, while for grain-displacing morphologies, only one such model exists in the literature. Thus the effect of morphology is poorly understood and this understanding is limited to pore-filling morphologies, despite the fact that grain-displacing hydrate inclusions will have a significant impact on the seismic signature of the sediment-hydrate system, and thus on the predicted quantity of hydrate. This paper presents a numerical modelling technique called computational homogenisation and applies it for the first time to gas hydrate-bearing sediments with grain-displacing morphologies. This technique has the ability to represent the geometry of hydrate inclusions explicitly and it considers the multi-scale nature of the material from a geotechnical engineering perspective. The effect of hydrate on the overall seismic properties of the host sediment is portrayed through simulations of nodular and simple vein morphologies with differing hydrate contents. Results show that morphology has a significant effect on the overall material properties, with the effect being more pronounced on the overall compressional wave velocity than on the overall shear wave velocity. The ratio of the two velocities ($V_p/V_s$) differs depending on the type of morphology and can be used to gain relevant insight by assisting in the differentiation between nodular and vein morphologies.

* Corresponding author: Phone: +44 (0)1125 320 600 E-mail: Gabrielle.Wojtowitz@burohappold.com
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NOMENCLATURE

E  Young’s modulus [MPa]
G  Shear modulus [MPa]
K  Bulk modulus [MPa]

V_p  Compressional wave velocity [m/s]
V_s  Shear wave velocity [m/s]

v  Poisson’s ratio

INTRODUCTION

Due to the metastable nature of gas hydrate, the identification of its in situ presence via the recovery of core samples has been problematic. Hence the presence and quantity of gas hydrate has been inferred via exploratory seismic surveys, which measure indirectly the bulk dynamic properties of sizeable volumes of sediment in situ. Seismic data are then interpreted using an effective medium model, which employs theoretical assumptions to relate wave velocities to gas hydrate content of the sediment. Wave velocity can then be used to infer hydrate concentration level.

Hydrates have been recovered in a variety of sediments ranging from fine-grained clays and silts to coarse-grained sands. The lithology of the host sediment influences the growth of gas hydrate and subsequently its morphology. The observed hydrate morphologies occur as two basic types, pore-filling and grain-displacing [1]. Pore-filling gas hydrate replaces pore fluid between sediment grains; whereas grain-displacing hydrate does not occupy sediment pore volume but instead forces grains apart forming layers, veins or nodules of pure gas hydrate. Grain-displacing morphologies occur over a wide range of sizes from thin micron thick veins to massive sheets of hydrate possibly metres in width. Graphical representations of typical grain-displacing hydrate morphologies are shown in Figure 1. Different morphologies will affect the physical properties of the host sediments in different ways and an understanding of this effect particularly for specific gas hydrate morphologies is important.

The relationship between morphology and structure of the sediment and the seismic signal is a key step in the process of remotely determining gas hydrate concentration and can be applied in an effective medium model used to interpret seismic data. A number of published effective medium models for gas hydrate-bearing sediments are available in the literature. The methods employ different techniques and assumptions with respect to hydrate morphology and are thus applicable for specific sediments. Of these methods it is unclear which to use to interpret seismically measured velocities as the methods predict quite different hydrate saturation estimates for the same data set and site [2,3,4,5]. A key factor in the application of effective medium models is the incorporation of the underlying hydrate morphology as well as the extent to which hydrate is assumed to contribute to the stiffness of the sediment.

In general the effective medium methods applied in the literature do not incorporate a detailed realistic representation of the microstructure and apply instead empirically determined parameters or assumptions with regards to the microstructural geometry or hydrate distribution in the sediment. Lee’s (1993) weighted equation [6] and the three-phase Biot theory [7] apply empirically determined parameters, which are site specific and cannot be transferred for application on other sites with different conditions. Other methods such as the three-phase effective medium method [8], four-phase Kuster-Toksoz model [9] and combined SCA-DEM method [10] apply different simplifying assumptions regarding the shapes of individual sediment components and the way they interact with each other. Due to these applied assumptions, the methods are limited to pore-filling hydrate morphologies only. In addition all the methods consider gas hydrate as finely, homogeneously and uniformly distributed in the host sediments.

Thus due to the assumptions upon which the methods are based, none of the approaches are
applicable for grain-displacing hydrate morphologies typically found in fine-grained sediments. Application of the existing methods to such sediments will yield misleading hydrate concentration estimates [5]. Methods that consider grain-displacing morphologies and their specific effect on the physical properties of hydrate-bearing sediments are rare. In the literature only one such method exists, this is the combined SCA-DEM method developed by Ghosh et al. (2010) [5]. This method is limited by the simplified assumptions it applies with regards to the shapes of the hydrate vein and nodular inclusions and cannot represent detailed, complex morphologies with a range of inclusion shapes and sizes.

It can be concluded that the effect of hydrate morphology on marine sediments is poorly understood and predominantly limited to pore-filling morphologies. This justifies the need for the development of a new modelling approach that can conceptualise and model more complex morphologies such as grain-displacing morphologies by taking geometry explicitly into account, thus complementing the existing models in the field by providing a means to investigate a larger range ofhydrate morphologies.

In this paper an alternative modelling approach for gas hydrate-bearing sediments based on first-order computational homogenisation is formulated for specific grain-displacing morphologies. The novelty of this approach is in its application of geotechnical engineering principles along with modelling techniques from material science, which have not been used in hydrate research to date. Computational homogenisation has the ability to represent inclusion geometry explicitly by considering the multi-scale nature of a material.

**COMPUTATIONAL HOMOGENISATION MODELLING APPROACH**


First-order computational homogenisation is a multi-scale method that is used in material science to model the mechanical response of heterogeneous materials, especially with the method of finite elements. Multi-scale approaches consider the material on different scales or levels of observation and are based on the fundamental assumption that the material is considered to be homogeneous on the macro-scale and heterogeneous on the micro-scale.

On the micro-scale, the actual geometric structure of the material is defined and the material properties for each individual constituent are defined explicitly. Whereas on the macro-scale the material is considered homogeneous and the material properties are the effective equivalent properties determined from the heterogeneous representation of the material on the micro-scale via an assumed micro-macro relationship or interaction [11,12,13,14]. This interaction between the two scales occurs by the coupling of the kinematics and the various stresses and forces in the two scales. Therefore the main idea is to bring the homogenised information of the detailed microstructural description to the macro-scale in the form of effective or overall material properties. A graphical illustration of the multi-scale computational homogenisation process is shown in Figure 2.

![Figure 2. Graphical representation of the multi-scale computational homogenisation modelling process (redrawn from [12]).](image)

In essence, first-order computational homogenisation consists of determining the constitutive response at a macro-scale point of a heterogeneous material, through the solution of a separate, appropriate boundary value problem formulated at the micro-scale. The strain and rotation at the macro-scale point are used to ‘drive’ the boundary conditions on the micro-volume, the microstructure of which is defined explicitly. The resulting stress increment field is averaged over the micro-volume, and it is applied as the stress increment at the corresponding macro-scale point.
In this work, the boundary value problem on the micro-scale is formulated by means of a representative volume element (RVE). The RVE should be large enough to contain sufficient information about the microstructure of the material but much smaller than the macroscopic body [15]. In this context, it is assumed that the wavelength of a propagating seismic wave is greater than the RVE. This in effect homogenises the material as the seismic wave ‘sees’ the overall material.

A hydrate morphology is assigned to the RVE and boundary value problems are solved yielding the effective elastic properties for this particular morphology. The boundary value problems are solved by means of a detailed finite element analysis, applying periodic boundary conditions and a load to the RVE. The resulting average stresses and strains determined from the analysis are used to calculate the elastic moduli of the material. Typical RVEs are shown in Figure 3.

Figure 3. Typical RVEs for (a) a nodular hydrate morphology corresponding to 37% hydrate content, (b) a parallel vein morphology corresponding to 50% hydrate content and (c) cross-cutting vein morphology corresponding to 46% hydrate content.

Periodic boundary conditions are applied to ensure the continuity of displacement and stress fields across the boundaries of the RVE and are applied to the boundary nodes of the RVE mesh in the form of constraint equations. The deformed shape of the RVE after the analysis can be used as a simple check for the correct application of periodic boundary conditions as opposite sides of the RVE should deform identically. This is shown in Figure 4 in the deformed RVE for simple shear.

It was confirmed that this assumed RVE is indeed “representative” by comparing the results to those of a larger model consisting of many RVEs stacked in a regular structure, and also to the response predicted for the same structure if the calculated (from the RVE) effective medium properties were used. All three results were equal indicating that the RVE is a valid representation of the material and the modelling procedure yields an appropriate set of average properties [16]. This is further supported by the good agreement between the results to those predicted with closed-form analytical approaches appropriate to the morphology used such as the Kuster-Toksoz (1974) model [17], Backus (1982) Upscaling [18] and Pariseau’s (1988) NRVE approach [19] [16].

Figure 4. Deformed RVE subjected to simple shear for a nodular hydrate morphology.

NUMERICAL MODELLING

Numerical analyses were conducted using the finite element software ABAQUS. Simple grain-displacing hydrate morphologies were considered consisting of nodules, parallel veins and cross-cutting veins. These morphologies were modelled as hydrate inclusions embedded in a host sediment matrix whereby the inclusions are represented by a geometric idealisation of their shape. A two-dimensional plane strain geometry was assumed. Thus hydrate nodules were modelled as cylindrical inclusions of different radii embedded in a host sediment matrix whereas hydrate veins of different thicknesses were idealised as prisms of different width and length. An example of a RVE for each of the morphologies is shown in Figure 3. The nodular hydrate morphologies were created using a random generator for different target hydrate contents, implemented in Matlab. The hydrate content was represented by the area occupied by the inclusions in relation to the total area of the RVE.
The modelled material represents a two-phase continuum and the overall effective macroscopic material behaviour is assumed to be linear elastic with perfect bonding between the material constituents. The overall material behaviour represented by each type of morphology is different due to their different geometry. The nodular morphology has an overall isotropic material behaviour. However the presence of veins makes a medium anisotropic with respect to wave propagation [20,21] and hydrate vein morphologies exhibit directionally dependent material behaviour. Parallel veins exhibit overall transversely isotropic material behaviour while cross-cutting veins exhibit orthorhombic behaviour.

Six-noded quadratic plane strain triangles were used in the finite element mesh. The properties of the constituent materials used in the analyses are shown in Table 1.

<table>
<thead>
<tr>
<th>Material</th>
<th>K (MPa)</th>
<th>G (MPa)</th>
<th>E (MPa)</th>
<th>ν</th>
</tr>
</thead>
<tbody>
<tr>
<td>Host sediment</td>
<td>490</td>
<td>188</td>
<td>500</td>
<td>0.33</td>
</tr>
<tr>
<td>Hydrate</td>
<td>7195</td>
<td>3000</td>
<td>7900</td>
<td>0.317</td>
</tr>
</tbody>
</table>

Table 1. Constituent material properties (where K represents bulk modulus, G, shear modulus, E, Young’s modulus, ν, Poisson’s ratio and bsf is below seafloor).

The results were represented by a normalised sediment bulk modulus value and normalised sediment shear modulus value. The normalised sediment modulus values were defined as the calculated modulus of the host sediment normalised by the modulus of pure hydrate. The material properties represented in Table 1 have a normalised bulk modulus of the host sediment of 0.068.

RESULTS AND DISCUSSION

For the investigated morphologies, a range of seismic wave velocities are predicted for a specific hydrate content depending on morphology and type of seismic wave. These are shown in Figures 6, 7 and 8 where the overall shear wave velocity ($V_s$), overall compressional wave velocity ($V_p$) and the ratio of the two velocities ($V_p/V_s$) are plotted as functions of hydrate content.

For low hydrate contents, less than 30%, the effect of the investigated morphologies on the overall shear wave velocity is insignificant, however as hydrate content increases, this effect becomes more pronounced. This is shown in Figure 6. Thus in practice when shear wave velocity is used for hydrate content prediction and low hydrate contents are inferred, for soft host sediments (to which a normalised bulk modulus of 0.068 corresponds) a smaller uncertainty (less than 6%) in predicted hydrate content is expected as compared with the greater uncertainty of 13% which is expected for hydrate contents greater than 30%.

A different effect is observed for compressional wave velocity. Compressional wave velocities are particularly dependent on directional material properties and the orientation of wave propagation with respect to vein orientation is important. This is shown in Figure 7 where for the same hydrate content and morphology, different compressional wave velocities occur. The data curve labelled Parallel 0 refers to parallel vein morphologies with a compressional wave propagating perpendicular to the veins and Parallel 90 refers to propagation parallel to the veins. This is shown schematically in Figure 5.

![Figure 5](image)

Figure 5. Schematic illustration of a parallel vein morphology with a compressional wave propagating (a) perpendicular to the veins ($0^\circ$ to the vertical) and (b) parallel to the veins ($90^\circ$ to the vertical).

For the morphologies investigated, when using compressional wave velocity for hydrate content prediction, an uncertainty in the hydrate content of approximately 37% is observed for soft host sediments (typically corresponding to a normalised bulk modulus of the host sediment of 0.068) if the specific underlying morphology and orientation of the wave propagation with respect to the vein inclination is unknown or inaccurately defined. Therefore the investigated morphologies clearly have a more pronounced effect on the overall compressional wave velocity than on the overall
shear wave velocity. Hence in practice for the prediction of hydrate content from seismic wave velocity data, a smaller uncertainty in the prediction would be obtained when using shear wave velocity.

Figure 6. Overall shear wave velocity computed from simulations of nodular, parallel vein and cross-cutting vein hydrate morphologies as a function of hydrate content for host sediment corresponding to a normalised sediment bulk modulus of 0.068 (where hydrate content is a percentage of the total area).

Figure 7. Overall compressional wave velocity computed from simulations of nodular, parallel vein and cross-cutting vein hydrate morphologies as a function of hydrate content for host sediment corresponding to a normalised sediment bulk modulus of 0.068 (where hydrate content is a percentage of the total area).

The overall compressional wave velocities corresponding to parallel vein morphologies form bounds within which the compressional wave velocities corresponding to nodular and cross-cutting vein morphologies fall. In practice, these bounds could be useful for constraining the expected hydrate contents for an observed overall compressional wave velocity or vice versa. For vein morphologies, if there is uncertainty regarding the specific underlying geometry or the direction of wave propagation in relation to the vein geometry, the bounds could be used to define the range of hydrate contents or compressional wave velocities that could be expected.

Figure 8. Ratio of overall compressional wave velocity to overall shear wave velocity computed from simulations of nodular, parallel vein and cross-cutting vein hydrate morphologies as a function of hydrate content for host sediment corresponding to a normalised sediment bulk modulus of 0.068 (where hydrate content is a percentage of the total area).

In Figure 8, the $V_p/V_s$ ratios corresponding to vein and nodular hydrate morphologies are plotted against hydrate content. For nodular morphology, the computed $V_p/V_s$ ratio was found to be approximately 2. This value is the same as that observed in the field for nodular hydrate morphologies [22] and can be predicted with a theoretical relationship. This relationship links the $V_p/V_s$ ratio to the Poisson’s ratio $\nu$ of the overall material and is only valid when the material is linear elastic, isotropic and homogeneous:

$$\frac{V_p}{V_s} = \sqrt{\frac{1-\nu}{0.5-\nu}} \quad (1)$$

However for vein morphologies, this relationship does not apply due to overall anisotropic material behaviour. For vein morphologies, the $V_p/V_s$ ratio is larger than that observed for nodular morphologies. Therefore in practice, if a larger $V_p/V_s$ ratio than that expected from the theoretical relationship is observed, it is possible that the underlying morphology has a vein-like structure. As observed for overall compressional wave
velocities, the $V_p/V_s$ ratios corresponding to parallel vein morphologies form a bounded range in which the $V_p/V_s$ ratios corresponding to crosscutting vein morphologies fall. Therefore if two compressional wave velocities taken at directions of wave propagation of 90° to each other can be measured, the two $V_p/V_s$ ratios determined from these two velocities can be used to constrain the range of ratios that are expected.

**CONCLUSIONS**

Computational homogenisation provides a means to model more complex hydrate morphologies, such as grain-displacing morphologies, by allowing the geometry of the micro-morphology to be modelled explicitly. Thus the effect of particular grain-displacing morphologies such as nodules and veins on the overall stiffness and seismic wave velocity of gas hydrate-bearing sediments can be investigated.

Results show that morphology has a significant effect on the overall material properties, with the effect being more pronounced on the overall compressional wave velocity than on the overall shear wave velocity. Knowledge of the particular underlying hydrate morphology will assist in constraining the estimation of hydrate content.

The ratio of the compressional and shear wave velocities ($V_p/V_s$) differs depending on the type of morphology and it appears that its value may provide insight into the underlying morphology by assisting in the differentiation between nodular and vein morphologies.

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