CFD Simulation of Low Reynolds-number Turbulence Models in Coral Thermal Microenvironment

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Abstract
The increasing frequency and severity of mass bleaching events in the past few decades has raised considerable concerns. Here we report on the numerical simulations of Low Reynolds turbulence models coral microenvironments to determine surface temperature rise in reef corals and test whether our model is capable to estimate of the extent of warming likely to be encountered in the nature during calm conditions. The Computational Fluid Dynamics (CFD) simulation uses the OPENFOAM CFD libraries to implement a steady-state turbulent flow porous medium model, with heat transfer accounted for using a transport equation for temperature. We validated the model using controlled laboratory experiment observations.

Introduction
Corals are one of the most ecologically and economically important habitat-forming species. However, they can bleach in response to stressful thermal conditions. The increasing frequency and severity of bleaching over the past few decades has raised considerable concern for the long-term viability of coral reefs. The combination of both elevated sea-surface temperature and solar irradiance is widely acknowledged to be the most important trigger for coral bleaching. Other environmental factors such as low flow, low salinity and low water turbidity can contribute to the bleaching responses by corals. These parameters vary considerably on coral species and morphologies, which can potentially determine the extent and variation of the fluid flow and mass and heat transfer in corals, and ultimately their susceptibility to bleaching.

The study of coral bleaching has been dominated by laboratory and field experiments, in-situ observations, and predictive modelling based on remotely sensed sea conditions. However, the reasons corals bleach are not fully understood. Laboratory studies can be confounded by sensitivity of most coral species to laboratory conditions and the difficulties inherent in accurately simulating the complexity and variability of oceanic conditions, while, field-based approaches are typically costly and are difficult to generalise from because of uncontrolled natural variation that may be relevant only to specific sites. Numerical methods on the other hand provide a powerful, holistic approach to solve physics associated with coral bleaching including a wide range of scales of fluid motion, heat transfer, and the morphology of the corals.

Conventionally, bleaching has been assessed on the basis of sea surface temperature (SST) data, however, it is the deviation of surface coral temperature from ambient SST, called thermal stress, that is most likely to trigger and determine the severity of bleaching. Previously, we established the potential of CFD in predicting the thermal stress imposed on corals by their thermal microenvironments under laminar flow conditions [1]. However, in the overwhelming majority of cases, the external flow stream carries with it a certain degree of turbulence. In essence, the laminar boundary layers are relatively easy to measure but in turbulent although there exists a very thin layer next to the wall called laminar or viscous sublayer, its thickness is so small that it is almost impossible or very difficult to observe under experimental conditions. Here we validate our computational predictions for the surface warming of corals that varied in pigmentation and validate our findings with the experimental observations [2].

Thermal regions in coral
Heat transfer within and around corals is affected by three main mechanisms: (1) the rate of incident radiation absorbed by the exposed tissue surface, (2) the rate of heat loss due to convection from the tissue and skeleton into the surrounding water, and (3) the rate of heat conduction from the tissue into the skeleton. The model presented here considers all of these mechanisms, with the tissue and skeleton layers each possessing slightly distinctive thermal properties. Although here we assumed that the living tissue is almost impermeable, however, in many cases, the activity of borers and coral grazers will result in openings allowing percolation and increased skeletal porosity.

Model validation
The experimental study of Fabricius et al. (2006) [2] was used to validate our turbulent CFD model. They conducted an experiment which exposed a range of different coral darkness (hemispherical coral (Favia matthaii), ≥90 nm) to direct sunlight ranging from high irradiance (1,500–1,600 μmol m⁻² s⁻¹ or ~800 W m⁻²) to low irradiance (120–350 μmol m⁻² s⁻¹ or ~150 W m⁻²) (Figure 1). Pigmentation was measured as background fluorescence, F0, which here defined as a proxy of a light-absorptivity coefficient where F0=100 as near white and F0=600 as dark brown. Measurements were taken outdoors in flow chambers (consisting of four 15-cm-deep and 45-cm-long working sections) creating an unidirectional flow with a steady inlet flow maintained at 0.01, 0.02, and 0.05 m s⁻¹ (only the latter flow speed was investigated since we are interested in validating the turbulence models, Re ≥ 4600), and a temperature of 29.3°C. Coral surface warming was given as the difference between coral surface temperature and ambient water temperature after a period of exposure to solar irradiance.
The mathematical model for steady, turbulent incompressible flow consists of the Reynolds average Navier-Stokes and energy equations. The continuity equation is given by

$$\frac{\partial \bar{u}_j}{\partial x_j} = 0 \quad (1)$$

where bar denotes a resolved or mean quantity. The averaged momentum equation is

$$\frac{\partial}{\partial x_j} (\bar{u}_i \bar{u}_j) = -\frac{\partial}{\partial x_i} \left( \frac{\bar{p}}{\rho} \right) + \frac{1}{\rho} \frac{\partial}{\partial x_j} (\tau_{ij} + \bar{S}_j) - \bar{S}_j \quad (2)$$

where $S_j$ is the flow sink term which can be divided into viscous and inertia effects [1]. The above equation is known as the Reynolds-Average Navier-Stokes equations (RANS), where $\tau_{ij}$ is the Reynolds-stress tensor and $\tau_{ij}$ is the mean laminar viscous stress and is given by

$$\tau_{ij} = \mu \left[ \left( \frac{\partial \bar{u}_i}{\partial x_j} + \frac{\partial \bar{u}_j}{\partial x_i} \right) - \frac{2}{3} \frac{\partial}{\partial x_k} \delta_{ij} \right] \quad (3)$$

where $\delta_{ij}$ is unit tensor and the second term contains $2/3$ multiplied by the divergence of velocity term is zero. The Reynolds-stress tensor represents the transfer of momentum due to turbulent fluctuations which is given by

$$\tau_{ij} = 2\mu_t S_{ij} - \frac{2}{3} \rho k \delta_{ij} \quad (4)$$

where $S_{ij}$ is the mean strain-rate tensor and $k$ is turbulent kinetic energy which is given as

$$k = \frac{1}{2} \bar{u}_i^2 = \frac{1}{2} \left( \bar{u}^2 + \bar{v}^2 + \bar{w}^2 \right) \quad (5)$$

The degree of turbulence can be adequately described using the intensity of turbulence, $I$, and the scale of turbulence, $l$. The energy equation is given by

$$\frac{\partial}{\partial x_j} (\bar{T} \bar{u}_j) = \frac{\partial}{\partial x_k} \left( \Gamma_{Teff} \frac{\partial \bar{T}}{\partial x_k} \right) - \frac{\alpha q}{\rho C_p} + \Phi \quad (6)$$

where $\Gamma_{Teff}$ is the effective thermal diffusivity $(\frac{\partial T}{\partial x} + \frac{\partial T}{\partial y})$, $\alpha$ is the tissue absorptivity, $q$ is the heat source due to irradiance, and $\Phi$ is turbulent heat dissipation fluxes $\left[ \frac{1}{2} \left( \frac{\partial \bar{w}_j}{\partial x_i} + \frac{\partial \bar{w}_i}{\partial x_j} + \frac{\partial \bar{w}_i}{\partial x_j} \right) \right]$, which has an effect on the temperature rise only for high Reynolds number cases.

### Setting grid

The models are able to resolve the viscous layer numerically by using very fine grids and viscous effects are included in the model by including ‘near wall damping’ terms. The low-Reynolds turbulence models are able to resolve the viscous layer numerically by using very fine grids and viscous effects are included in the model by including ‘near wall damping’ terms. Typically, this requires ensuring the near-wall cell at non-dimensional distance of $y^+ \leq 1$.

$$y^+ = \frac{y v u^*}{\nu} \quad (7)$$

$$\tau_{aw} = C_f \frac{\rho U_0^2}{2} \quad (8)$$

where $y$ is the actual distance from the wall, $u^*$ is the friction velocity, and $\tau_{aw}$ is the wall shear stress.

### Boundary conditions

To adequately accommodate the flow conditions corresponding to the experiment, it was necessary to specify free stream boundary conditions. We estimated the turbulence intensity, $I$, and length scale, $l$ to be $\sim 0.5-1\%$ and $\sim 20-40\%$ of coral diameter, respectively. The free-stream turbulence variables can be computed from the following Table 1 and 2, where $C_p$ represents a constant of 0.09. To impose boundary layers in the viscous sublayer region and to accommodate convergence, the initial conditions of $k$ and $\omega$ at the wall are specified differently from the free-stream conditions. The rest of bounding boundaries are set as symmetry plane which applies zero gradient condition for scalars except for vectors and tensor fields. The boundary conditions applied at the inlet for $k$, $\varepsilon$, and $\omega$ were used to define the turbulent kinetic energy, dissipation, and frequency from both the fraction of the mean velocity and the mixing length.

### Table 1: Free-stream specification

<table>
<thead>
<tr>
<th>Parameter</th>
<th>formula</th>
</tr>
</thead>
<tbody>
<tr>
<td>$k$</td>
<td>$\frac{1}{2} \left( U_i^2 \right)$</td>
</tr>
<tr>
<td>$\varepsilon$</td>
<td>$\frac{C_p k^{-1/4} \sqrt{\kappa}}{\nu}$</td>
</tr>
<tr>
<td>$\omega$</td>
<td>$C_p^{-1/4} \sqrt{\kappa}$</td>
</tr>
<tr>
<td>$\omega_{wall}$</td>
<td>$\frac{600 \nu}{\nu}$</td>
</tr>
</tbody>
</table>

### Table 2: Boundary conditions

<table>
<thead>
<tr>
<th>Parameter</th>
<th>floor</th>
<th>inlet</th>
<th>outlet</th>
</tr>
</thead>
<tbody>
<tr>
<td>$k$ (m$^2$s$^{-2}$)</td>
<td>FV</td>
<td>TKI</td>
<td>IO</td>
</tr>
<tr>
<td>$\varepsilon$ (m$^2$s$^{-3}$)</td>
<td>FV</td>
<td>TDI</td>
<td>IO</td>
</tr>
<tr>
<td>$\omega$ (s$^{-1}$)</td>
<td>FV</td>
<td>TFI</td>
<td>IO</td>
</tr>
<tr>
<td>$u$ (m s$^{-1}$)</td>
<td>NS</td>
<td>FV</td>
<td>IO</td>
</tr>
<tr>
<td>$T$ (K)</td>
<td>FV</td>
<td>FV</td>
<td>ZG</td>
</tr>
</tbody>
</table>

*ZG: zero gradient, FV: fixed value, NS: non-slip, TKI: turbulent intensity kinetic energy inlet, TDI: turbulent mixing length dissipation rate inlet, TFI: turbulent mixing length frequency inlet
Numerical schemes

The schemes implemented for both convection divergence and Laplacian terms were the Gauss linear upwind cell limited least squares and the Gauss linear limited 0.5, respectively. The generalised geometric-algebraic multi-grid (GAMG), smoother Gauss-Seidel, and preconditioned bi-conjugate gradient (PBICG) were used to discretised pressure, velocity, and temperature governing equations, respectively. The semi-implicit method for pressure-linked equation (SIMPLE) algorithm, which calculates the pressure on a staggered grid from velocity components by applying an iterative procedure coupled with the Navier-Stokes equations.

Results and Discussion

Due to the absence of real experimental measurements of axial velocity and wall shear stress at the upstream of the outlet, here we only validate the turbulence models based on the heat transfer performance of measured coral surface warming distribution. In this study, four of the most popular Low-Reynolds-number models were selected in the benchmark comparisons - the two equations \( k - \varepsilon \) SST, the two equation \( k - \omega \) model Launder-Sharma, the two equations \( k - \omega \), and the one-equation model Spalart-Allmaras (Figure 2, 3, and 4). The \( k - \omega \) SST and \( k - \varepsilon \) Launder-Sharma models both give good agreements with the experimental data and are much less dissipative which results in higher values of calculated velocity. These two models tended to establish downstream laminar flow when the free-stream turbulence level is low \( \left( \frac{U_{rms}}{U_{*}} \right) \leq 0.1 \) [5]. We briefly compared the sensitivity of the four models to free stream turbulent quantities and wall spacings. The results of the Spalart-Allmaras model show a reasonable agreement with the experimental data and insensitive to the free stream intensity values ranging from 1-15%. The two-equation models exhibits stronger sensitivity towards the turbulence levels in that the solutions tended to be laminar when the free stream levels were low, and vice versa [5]. We briefly investigated the wall spacing sensitivity to the turbulence models by varying the \( y^+ \) spacings of 0.1 and 0.25; and all the models yields similarly consistent results for the shear stress.

Our results demonstrate that the magnitude of temperature rise in coral tended to increase linearly with increasing pigmentation/absorptivity (Figure 1). Our prone estimates of irradiance absorbed for each pigmented corals \( F(0, \text{coral, darkness}) \) could have implications for under-predicting the overall coral surface warming (Figure 2). The mean and standard deviation of the low irradiance and high irradiance experimental results are 0.267±0.094 (99.7% confidence intervals: -0.015 to 0.549) 0.457±0.232 (99.7% confidence intervals: -0.239 to 1.153), respectively. The root mean squared error (RMSE) for each of the models associated with the experimental results is reported in Table 3.

![Figure 2: Effects of flow, irradiance, and pigmentation on coral surface warming at low irradiance](image)

![Figure 3: Effects of flow, irradiance, and pigmentation on coral surface warming at high irradiance](image)

<table>
<thead>
<tr>
<th>RMSE (K)</th>
<th>( k - \omega ) SST</th>
<th>( k - \omega )</th>
<th>( k - \varepsilon ) L-S</th>
<th>S-A</th>
</tr>
</thead>
<tbody>
<tr>
<td>Low irradiance</td>
<td>0.433</td>
<td>0.823</td>
<td>0.152</td>
<td>0.561</td>
</tr>
<tr>
<td>High irradiance</td>
<td>0.273</td>
<td>1.033</td>
<td>0.154</td>
<td>0.361</td>
</tr>
</tbody>
</table>

Conclusion

In summary, we have demonstrated that CFD technique is a powerful tool for determining the physical mechanisms of thermal stress in coral microenvironment at turbulent regime, which would have been otherwise difficult to observe by experimental means.

Acknowledgement

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References


[3] Launder, BE and Sharma, BI, Application of the energy-dissipation model of turbulence to the calculation of flow
Figure 4: Slices of axial velocity and temperature profiles at low irradiance at $F_0=100$


