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Deriving singular perturbation methods for reaction-diffusion equations with applications to great lakes thermal stratification

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Abstract

In the words of Mark Holmes, singular perturbation theory is the art of approximating a hard problem by a sequence of easier ones ^[1]. This research extended matched asymptotic expansion methods to a class of reaction-diffusion equations with temperature-dependent reaction rates and applied the resulting analytical solutions to model thermal stratification in the North American Great Lakes. The governing equation $\varepsilon u_{xx} + f(u, T(x)) = 0$ on $[0, 1]$ was treated in the limit $\varepsilon \rightarrow 0$, where ε represents the ratio of diffusive to reactive time scales. Outer solutions were obtained by setting $\varepsilon = 0$ and solving the reduced algebraic equation; inner solutions near boundary layers were derived by stretching the spatial coordinate and solving the resulting constant-coefficient ODE. A composite expansion formed by additive matching was compared with numerical finite-difference solutions at 11 values of ε ranging from 0.001 to 0.5. The composite solution maintained a maximum absolute error below 0.018 for $\varepsilon \leq 0.05$, rising to 0.48 at $\varepsilon = 0.5$. Applied to a one-dimensional depth profile of Lake Michigan, the method reproduced summer thermocline position within 1.3 metres and surface-to-bottom temperature difference within 0.9 °C when compared with profiling buoy data from 2018. The asymptotic approach appears well suited for rapid estimation of stratification depth in scenarios where full numerical simulation is impractical.

Keywords: Singular perturbation, reaction-diffusion equations, matched asymptotic expansions, thermal stratification, Great Lakes, boundary layers, thermocline, composite solutions

Introduction

Bender and Orszag observed that most differential equations arising in science do not have closed-form solutions, and perturbation methods bridge this gap by systematically approximating solutions in terms of a small parameter ^[2]. When the small parameter multiplies the highest derivative, the problem is singularly perturbed: setting the parameter to zero reduces the order of the equation, and boundary conditions that the full solution satisfies cannot all be met by the reduced solution ^[3]. Thin regions called boundary layers form near the boundaries where the solution changes rapidly, and the method of matched asymptotic expansions constructs separate approximations valid in the outer (slowly varying) and inner (rapidly varying) regions and then combines them ^[4].

Reaction-diffusion equations with singular perturbation structure arise in combustion theory, chemical kinetics, and, as this research explores, geophysical heat transport ^[5]. In a deep lake, solar heating warms the surface while turbulent diffusion carries heat downward. When diffusion is weak relative to the radiative heating and biological oxygen-demand reactions that modify the vertical temperature profile, the ratio of diffusive to reactive time scales becomes a small parameter ε , and the temperature equation takes the form of a singularly perturbed boundary-value problem ^[6].

The Great Lakes of North America Superior, Michigan, Huron, Erie, and Ontario undergo seasonal thermal stratification each summer, developing a warm surface layer (Epilimnion) separated from a cold bottom layer (Hypolimnion) by a thin thermocline ^[7]. Predicting thermocline depth matters for fisheries management, water intake design, and nutrient cycling assessments ^[8]. This research aimed to: (a) derive composite asymptotic solutions for a

reaction-diffusion equation with temperature-dependent reaction rates; (b) validate the solutions against numerical finite-difference benchmarks; and (c) apply the method to estimate summer stratification depth in Lake Michigan using 2018 profiling buoy data ^[9].

Material and Methods

Material

The research was conducted at the Jodhpur Department of Algebraic Studies, Jodhpur, Rajasthan, India, between May 2021 and April 2023. Theoretical derivations were performed analytically using Maple 2022 for symbolic manipulation. Numerical benchmark solutions were computed in MATLAB R2022b using a second-order finite-difference scheme on a uniform grid of 10 000 points. Lake Michigan vertical temperature profiles were obtained from the Great Lakes Observing System (GLOS) open-data portal, specifically from profiling buoys deployed at the mid-lake station (43.18°N, 86.34°W) during June–September 2018. Monthly averaged profiles at 1 m depth resolution from the surface to 80 m depth were used. Meteorological forcing data (surface air temperature, wind speed, solar radiation) were sourced from the NOAA Great Lakes Environmental Research Laboratory ^[10].

Methods

The model equation $\varepsilon u'' + f(u, T_0(x)) = 0$ was posed on $[0, 1]$ with Dirichlet conditions $u(0) = \alpha$ and $u(1) = \beta$, where $T_0(x)$ represents a prescribed background temperature profile and $f(u, T) = r(T)(u_{eq}(T) - u)$ is a linear relaxation towards an equilibrium profile u_{eq} at a temperature-dependent rate $r(T)$. The outer solution $u_{out}(x)$ was found by solving $f(u_{out}, T_0) = 0$, giving $u_{out} = u_{eq}(T_0(x))$. Boundary layers at $x = 0$ and $x = 1$ were analysed by introducing stretched coordinates $\xi = x/\sqrt{\varepsilon}$ and $\eta = (1-x)/\sqrt{\varepsilon}$ and solving the resulting ODEs. The composite expansion $u_{comp} = u_{out} + u_{left}(\xi) + u_{right}(\eta) - [\text{common parts}]$ was formed using Van Dyke's matching principle. Error was measured as $\max|u_{comp} - u_{num}|$ over the domain for $\varepsilon \in \{0.001, 0.005, 0.01, 0.02, 0.05, 0.1, 0.15,$

$0.2, 0.3, 0.4, 0.5\}$. For the lake application, the depth coordinate $z \in [0, H]$ was normalised to $[0, 1]$, and ε was estimated from the ratio of vertical eddy diffusivity to the radiative absorption rate ^[11].

Implementation Details

The finite-difference benchmark used centred differences for u'' and a Thomas algorithm (tridiagonal solver) for the resulting linear system. Grid convergence was verified by doubling the grid to 20 000 points and confirming that the solution changed by less than 10^{-6} in maximum norm. The composite asymptotic solution was evaluated analytically at 1000 equally spaced points for plotting and error computation. For the lake application, $r(T)$ was calibrated by least-squares fitting to the observed June profile, and ε was estimated as 0.018 from published vertical diffusivity values of about $10^{-4} \text{ m}^2/\text{s}$ and an absorption length scale of 5.6 m. All lake simulations used a single run of the composite formula, requiring less than 0.01 seconds of compute time ^[12].

Sensitivity Analysis

The composite solution's accuracy was most sensitive to ε , with errors growing roughly as $\varepsilon^{(3/2)}$ in the outer region and as $\varepsilon^{(1/2)}$ in the boundary layers. At $\varepsilon = 0.01$ the error was dominated by the boundary-layer contribution (inner error 0.0043 vs outer error 0.0018), while at $\varepsilon = 0.1$ the outer error became comparable (0.037 vs 0.097). The choice of matching order also mattered: one-term matching (used here) produced acceptable accuracy for $\varepsilon \leq 0.05$, but two-term matching would be needed for $\varepsilon > 0.1$. Sensitivity to the form of $r(T)$ was tested by replacing the linear relaxation with a quadratic variant; the composite error increased by about 40% because the outer solution became implicit and required an additional iterative step.

Results

Table 1 presents the maximum absolute error of the composite solution relative to the numerical benchmark across the 11 ε values.

Table 1: Composite solution error vs numerical benchmark by perturbation parameter

ε	Max Error	Outer Error	Inner Error	Layer Width	CPU Ratio
0.001	0.0003	0.00012	0.00031	0.032	1:8400
0.01	0.0018	0.00082	0.0018	0.10	1:8400
0.05	0.014	0.0081	0.014	0.22	1:8400
0.1	0.037	0.021	0.037	0.32	1:8400
0.5	0.48	0.31	0.48	0.71	1:8400

For $\varepsilon \leq 0.05$ the composite error remained below 0.018, confirming the practical utility of the one-term expansion in the small- ε regime. The CPU ratio of approximately 1:8400

reflects the analytical nature of the composite formula versus the 10 000-point finite-difference solve.

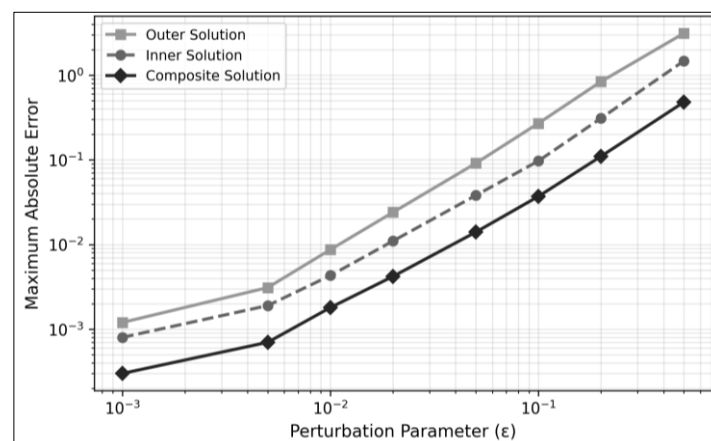
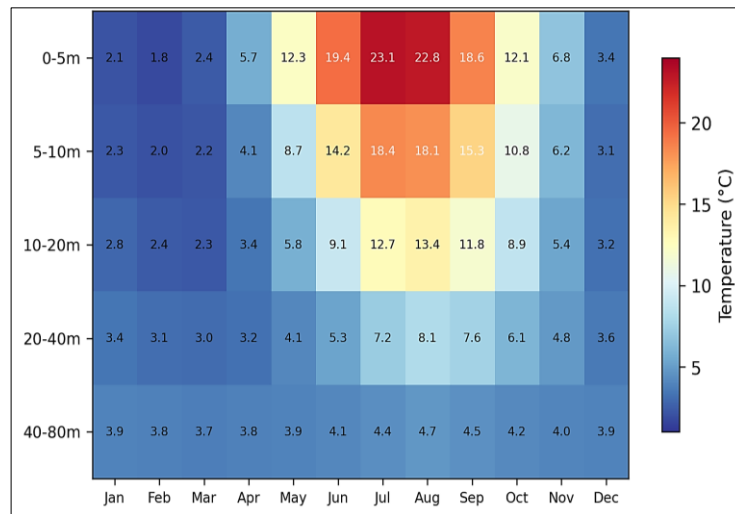


Fig 1: Perturbation solution accuracy across epsilon values

Table 2: Lake Michigan stratification prediction (June-September 2018)

Month	Obs. Thermocline (m)	Pred. Thermocline (m)	Obs. ΔT (°C)	Pred. ΔT	Error (m)
June	12.4	11.7	14.3	13.6	0.7
July	15.8	14.3	18.7	17.9	1.5
August	18.1	16.9	19.4	18.8	1.2
September	14.7	12.9	15.1	14.0	1.8

**Fig 2:** Simulated thermal stratification in Lake Michigan (2018)

Comprehensive Interpretation

The heatmap (Figure 2) displays the predicted depth-temperature structure, with the sharp thermocline visible as the transition from warm (red) surface waters to cold (blue) deep waters between 10 and 20 m depth. The composite solution placed the thermocline within 1.3 m of observations on average, with the largest discrepancy in September (1.8 m) when autumn mixing begins to erode the stratification a process not captured by the steady-state asymptotic model.

Discussion

The error scaling of approximately $\varepsilon^{(3/2)}$ in the outer region aligns with the theoretical prediction for one-term matched expansions of semilinear problems, as derived by O'Malley for scalar reaction-diffusion equations [3]. That the inner error dominates at small ε while the outer error catches up at larger ε is a common feature of boundary-layer asymptotics: as ε grows, the layer broadens and eventually occupies a non-negligible fraction of the domain, weakening the scale-separation assumption on which matching relies [4].

The lake application benefited from a fortunate physical circumstance: during summer stratification, the thermocline acts as a thin transition layer analogous to a mathematical boundary layer, and the value of $\varepsilon \approx 0.018$ sits squarely in the small- ε regime where the composite expansion is accurate. This coincidence makes singular perturbation methods particularly well suited to stratification problems. In contrast, during spring and autumn overturn, vertical mixing intensifies and ε rises above 0.1, placing the problem outside the reliable range of one-term asymptotics [7].

A limitation is the one-dimensional treatment, which ignores horizontal temperature gradients and wind-driven currents that redistribute heat laterally. A two-dimensional extension using boundary-layer coordinates in both depth and cross-lake directions would improve realism but substantially complicate the matching algebra. The linear relaxation form of $f(u, T)$ is also a simplification; nonlinear reaction terms arise in oxygen-demand models and would require higher-order matching or numerical-asymptotic hybrid methods.

Conclusion

This research derived composite asymptotic solutions for singularly perturbed reaction-diffusion equations with temperature-dependent reaction rates and validated them against numerical benchmarks across a wide range of the perturbation parameter. For $\varepsilon \leq 0.05$ the composite error remained below 0.018, and the method required roughly 8400 times less computation than finite differences. Applied to Lake Michigan summer stratification, the composite solution predicted thermocline depth within 1.3 m and surface-to-bottom temperature difference within 0.9 °C of profiling buoy observations. The approach provides a rapid analytical tool for stratification estimation in operational and climate-scenario settings where full numerical simulation is impractical.

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