

**LAGRANGIAN PARTICLE TRACKING BASED SIMULATION OF
ANOMALOUS HYDRODYNAMIC TRANSPORT THROUGH SHALLOW
WATER LAKES WITH CROWDING: IMPLICATION FOR
CONSERVATION STRATEGIES**

ARVIND KUMAR BAIRWA



**DEPARTMENT OF CIVIL ENGINEERING
INDIAN INSTITUTE OF TECHNOLOGY DELHI**

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by

ARVIND KUMAR BAIRWA

DEPARTMENT OF CIVIL ENGINEERING

Submitted

in fulfillment of the requirements of the degree of Doctor of Philosophy

to the



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JULY 2024

Dedicated To
My Supervisor and My Mother

Certificate

This is to certify that the thesis, titled “Lagrangian Particle Tracking Based Simulation of Anomalous Hydrodynamic Transport Through Shallow Water Lakes With Crowding: Implication for Conservation Strategies”, being submitted by Mr. Arvind Kumar Bairwa to the Indian Institute of Technology, Delhi, for the award of Doctor of Philosophy, is a record of bonafide research work carried out by him under our joint-supervision. In our opinion, the thesis work has reached the standard, fulfilling the requirements for the said degree. Further, we certify that this submission is Mr. Arvind’s work and that, to the best of our knowledge and belief, it contains no material previously published or written by another person which, to a substantial extent, has been accepted for the award of any other degree or diploma of any University or Institute, except where due acknowledgment has been made in the text.

Prof Rakesh Khosa

Prof. R.Maheswaran

Professor (Retd.),

Department of Civil Engineering

Department of Civil Engineering

Indian Institute of Technology Hyderabad

Indian Institute of Technology Delhi

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Arvind Kumar Bairwa

Abstract

The efficient mixing and spreading of the contaminants are desirable for the health of the shallow-water lake ecosystem. The tracer spreading implies how long the Lagrangian parcel takes to exit the water body, whereas mixing encodes how quickly the flow dilutes the tracer concentration gradient. In shallow water lakes, the hydrodynamic transport of nutrients is often hindered by various random arrangements of dense packing bluff bodies, such as vegetative patches, garbage clusters, and circular cage farm rings. These configurations can profoundly affect the spatial velocity distribution by creating stagnation and dead zone regions, which can consequently negatively impact the health of the shallow water body by influencing the mixing and spreading of nutrients. Therefore, an objective understanding of hydrodynamic transport through the crowded media in shallow water lakes is crucial to developing potentially sound conservation, preservation, and restoration-related management paradigms for shallow water lakes.

Traditionally, almost all the research in flow through a crowded media has been focused on computing Eulerian quantities such as drag coefficient and turbulent fluctuations. These measures provide poor insight into the transport of fluid parcels because scalar mixing and transport is entirely a Lagrangian concept. In addition, transport through crowded media is often modeled using the classical advection-dispersion equation (ADE) model, and while incredibly powerful, a key limitation of such approaches is that they are, strictly speaking, only valid at late or asymptotic times, meaning after times when the solute has had enough time to sample the full distribution of velocities. This is quantified by the timescale $\tau_\kappa = l^2/\kappa$, where l is the domain characteristic length and κ is the diffusion coefficient of the solute. At pre-asymptotic times, i.e. less than τ_κ it is typically observed that the second centered moment grows superdiffusively in time (faster than linear growth in time), an observation that classical ADE with constant dispersion coefficient cannot reproduce.

To investigate mixing and anomalous transport, two distinct numerical scenarios of an array of circular cylinders viz without and with channels are designed. The finite-time Lyapunov exponent (FTLE) diagnostic approach is used to understand the mixing in the crowded domain. In the first scenario, an array of cylinders gradually increases, and FTLE is investigated with particle tracking simulation. As the solid volume fraction (SVF) increases with decreasing cylinder spacing, the

mixing worsens due to the poor stirring strength of the cylinder elements in the array. In contrast, mixing gets enhanced by introducing channels in the crowded media (second case) due to the formation of coherent structures at the channel-cylinder array interface.

To test anomalous (non-Fickian) transport in crowded media, two metrics, mean square displacement (MSD) and travel time distribution (TTD), are studied. As the Reynold number increases, the Fickian regime emerges very late, passing through a super-diffusive regime. In addition, TTD also exhibits a power law tail, suggesting that tracer traps in the recirculation region for an extremely long time before exiting the domain. This implies that MSD evolves non-linearly with time in the pre-asymptotic regime and ADE with a constant effective dispersion coefficient cannot be applied to model anomalous transport in crowded media.

Finally, a fractional advection-diffusion, a.k.a continuous time random walk (CTRW), is studied to model anomalous transport. The simulated TTD obtained in the scenario ‘with channel’ is used to validate the efficacy of the CTRW and ADE model at the Reynolds number spanning from steady to unsteady regime. It is observed that the CTRW model effectively predicts the effects of cylinder-scale flows on tracer transport, whereas the ADE model fails to capture the tailing effect. We conclude that the CTRW model should be preferred when modeling transport through dense, crowded media.

Keywords: Lagrangian particle tracking, Finite-time Lyapunov exponent, Travel time distribution, Anomalous transport, Continuous time random walk model

अमूर्त

उथले पानी वाली झील पारिस्थितिकी तंत्र के स्वास्थ्य के लिए दूषित पदार्थों का कुशल मिश्रण और प्रसार वांछनीय है। ट्रेसर प्रसार से पता चलता है कि लैंग्रेजियन पार्सल को जल निकाय से बाहर निकलने में कितना समय लगता है, जबकि मिश्रण एनकोड करता है कि प्रवाह कितनी तेजी से ट्रेसर एकाग्रता ढाल को पतला करता है। उथले पानी की झीलों में, पोषक तत्वों का हाइड्रोडायनामिक परिवहन अक्सर घने पैकिंग ब्लफ़ निकायों की विभिन्न यादृच्छिक व्यवस्थाओं, जैसे वनस्पति पैच, कचरा क्लस्टर और गोलाकार पिंजरे फार्म रिंगों से बाधित होता है। ये विन्यास ठहराव और मृत क्षेत्र क्षेत्रों का निर्माण करके स्थानिक वेग वितरण को गहराई से प्रभावित कर सकते हैं, जिसके परिणामस्वरूप पोषक तत्वों के मिश्रण और प्रसार को प्रभावित करके उथले जल निकाय के स्वास्थ्य पर नकारात्मक प्रभाव पड़ सकता है। इसलिए, उथले पानी की झीलों में भीड़ भरे मीडिया के माध्यम से हाइड्रोडायनामिक परिवहन की एक उद्देश्यपूर्ण समझ उथले पानी की झीलों के लिए संभावित रूप से ध्वनि संरक्षण, संरक्षण और बहाली-संबंधी प्रबंधन प्रतिमानों को विकसित करने के लिए महत्वपूर्ण है।

परंपरागत रूप से, भीड़ भरे मीडिया के माध्यम से प्रवाह में लगभग सभी शोध यूलेरियन मात्राओं जैसे ड्रैग गुणांक और अशांत उतार-चढ़ाव की गणना पर केंद्रित रहे हैं। ये उपाय द्रव पार्सल के परिवहन में खराब अंतर्दृष्टि प्रदान करते हैं क्योंकि स्केलर मिश्रण और परिवहन पूरी तरह से एक लैंग्रेजियन अवधारणा है। इसके अलावा, भीड़ भरे मीडिया के माध्यम से परिवहन को अक्सर शास्त्रीय संवहन-फैलाव समीकरण (एडीई) मॉडल का उपयोग करके तैयार किया जाता है, और अविश्वसनीय रूप से शक्तिशाली होते हुए भी, ऐसे दृष्टिकोणों की एक प्रमुख सीमा यह है कि वे, सख्ती से बोलते हुए, केवल देर से या स्पर्शोन्मुख समय पर मान्य होते हैं, जिसका अर्थ है ऐसे समय के बाद जब विलेय के पास वेगों के पूर्ण वितरण का नमूना लेने के लिए पर्याप्त समय हो। इसे टाइमस्केल $\tau_K = 12/K$ द्वारा निर्धारित किया जाता है, जहां 1 डोमेन विशेषता लंबाई है और K विलेय का प्रसार गुणांक है। प्री-एसिम्प्टोटिक समय पर, यानी τ_K से कम, यह आम तौर पर देखा जाता है कि दूसरा केंद्रित क्षण समय में अतिविस्तारित रूप से बढ़ता है (समय में रैखिक वृद्धि की तुलना में तेज़), एक अवलोकन जिसे निरंतर फैलाव गुणांक के साथ एक प्रभावी एडीई द्वारा पुनः उत्पन्न नहीं किया जा सकता है।

मिश्रण और असामान्य परिवहन की जांच करने के लिए, गोलाकार सिलेंडरों की एक श्रृंखला के दो अलग-अलग संख्यात्मक परिदृश्य तैयार किए गए हैं, जैसे कि चैनल के बिना और चैनल के साथ। भीड़-भाड़ वाले क्षेत्र में मिश्रण को समझने के लिए परिमित-समय ल्युपुनोव प्रतिपादक (एफटीएलई) निदान दृष्टिकोण का उपयोग किया जाता है। पहले परिदृश्य में, सिलेंडरों की एक श्रृंखला धीरे-धीरे

बढ़ाई जाती है, और कण ट्रेकिंग सिमुलेशन के साथ एफटीएलई की जांच की जाती है। जैसे ही सिलेंडर की दूरी कम होने के साथ ठोस आयतन अंश (एसवीएफ) बढ़ता है, सरणी में सिलेंडर तत्वों की खराब सरगर्मी शक्ति के कारण मिश्रण खराब हो जाता है। इसके विपरीत, चैनल-सिलेंडर सरणी इंटरफ़ेस पर सुसंगत संरचनाओं के गठन के कारण भीड़ भरे मीडिया (दूसरे मामले) में चैनल पेश करने से मिश्रण बढ़ जाता है।

भीड़-भाड़ वाले मीडिया में विषम (गैर-फ़िकियन) परिवहन का परीक्षण करने के लिए, दो मैट्रिक्स, माध्य वर्ग विस्थापन (एमएसडी) और यात्रा समय वितरण (टीटीडी) का अध्ययन किया जाता है। यह देखा गया है कि जैसे-जैसे रेनॉल्ड संख्या बढ़ती है, फ़िकियन शासन बहुत देर से उभरता है, एक सुपर-डिफ्यूसिव शासन से गुजरता है। इसके अलावा, टीटीडी एक पावर लॉ टेल भी प्रदर्शित करता है, जो सुझाव देता है कि ट्रेसर डोमेन से बाहर निकलने से पहले बहुत लंबे समय तक रीसर्क्युलेशन क्षेत्र में फंसा रहता है। इसका तात्पर्य यह है कि एमएसडी प्री-एसिम्प्टोटिक शासन में समय के साथ गैर-रैखिक रूप से विकसित होता है, और निरंतर प्रभावी फैलाव गुणांक वाले एडीई को भीड़ भरे मीडिया में विषम परिवहन के मॉडल पर लागू नहीं किया जा सकता है।

अंत में, एक भिन्नात्मक संवहन-प्रसार, अर्थात् निरंतर समय यादृच्छिक चलना (CTRW), का अध्ययन विसंगतिपूर्ण परिवहन को मॉडल करने के लिए किया जाता है। 'चैनल के साथ' परिदृश्य में प्राप्त सिम्युलेटेड टीटीडी का उपयोग स्थिर से अस्थिर शासन तक फैले रेनॉल्ड्स नंबर पर सीटीआरडब्ल्यू और एडीई मॉडल की प्रभावकारिता को सत्यापित करने के लिए किया जाता है। यह देखा गया है कि सीटीआरडब्ल्यू मॉडल ट्रेसर ट्रांसपोर्ट पर सिलेंडर-स्केल प्रवाह के प्रभावों की प्रभावी ढंग से भविष्यवाणी करता है, जबकि एडीई मॉडल टेलिंग प्रभाव को पकड़ने में विफल रहता है। हम यह निष्कर्ष निकालते हैं कि घने, भीड़ भरे मीडिया के माध्यम से परिवहन मॉडलिंग में सीटीआरडब्ल्यू मॉडल को प्राथमिकता दी जानी चाहिए।

कीवर्ड: लैंग्रेंजियन कण ट्रेकिंग, परिमित समय ल्युपुनोव प्रतिपादक, यात्रा समय वितरण, विषम परिवहन, निरंतर समय यादृच्छिक वॉक मॉडल

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Acronyms and Abbreviations

1D	One Dimensional
2D	Two Dimensional
ADE	Advection diffusion equation
BTC	Breakthrough curve
CTRW	Continuous time random walk
CLT	Central limit theorem
DNS	Direct numerical simulation
FPT	First passage time
FTLE	Finite time Lyapunov exponent
LCSs	Lagrangian coherent structures
LPT	Lagrangian particle tracking
L.H.S	Left-hand side
MSD	Mean square displacement
MFPT	Mean first passage time
Q-criterion	Q-criterion
R.H.S	Right-hand side
TPL	Truncated power law
TTD	Travel time distribution