Activity-Induced Mixing in a Stratified Binary Passive System

Thomas Jacob, Siddhant Mohapatra, and Pallab Sinha Mahapatra

Abstract Active systems have garnered interest from researchers worldwide for their fascinating displays of congregations and the far-reaching scope of biomimetic applications. The current chapter talks about one such application: the use of active particles to induce mixing in a stratified passive system. Simulations using a Langevin model in two dimensions shows the mixing state of the initially stratified system reach a saturation point in finite time. Interestingly, with change in the number of active mixers, only the rate of mixing is found to be affected, while the final mixed state is perceived to be almost similar. Active particles numbering not more than 20% of that of the passive species is found to be enough to induce brisk mixing. An investigation is parallelly carried out into the maximum rotation allowed for each active mixer to maximise the overall mixing effect. The objective of this discourse is to provide a numerical backbone to the feasibility of the use of micro/mini robots for mixing of living/non-living entities, while also discussing the factors affecting the process.

Keywords Active–passive system · Mixing · Gini coefficient · Over-damped Langevin model

1 Introduction

Researchers have always been amused by the pattern formation in schools of fish, swarms of bees, flocks of starlings, armies of ants, etc. The curiosity about the underlying processes leading to such intricate phenomenon have motivated the study and evolution of active matter systems. Such systems continuously consume energy for their activity and hence, are always out of equilibrium. Researchers have been trying to capture and accurately decode the behaviour of such active entities since the last few decades and in the recent years, the advent of high-speed computing facilities has aided the process by allowing large-scale numerical modelling of the active

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systems with a high temporal and spatial resolution. Some notable mathematical models proposed to mimic these active systems are the Vicsek model [1], the Active Brownian Particle model [2], the Run and Tumble model [3] among others.

The interaction between active (those with the ability to self-propel) and passive (those which cannot self-propel) particles have been a centre of attention for researchers due to intriguing behaviour such as segregation [4], Motility Induced Phase Separation (MIPS) [5], cluster formation [6], etc. The upcoming section discusses several works highlighting the dynamics of such systems with dispersity in motility.

2 Literature Review and Objective

The study of active matter systems was initially pursued from a numerical viewpoint during the 1990s with the advent of various mathematical models [7]. Since then, there has been extensive research in the field using both experimental and computational methods. Even though active matter systems evolved after observing behavioural patterns in living systems, there are reported studies where interactions could also be observed among active (both living & artificial) and passive particles (particles with no activity) in a pool [8, 9]. One of the major limitations with experiments in the field comes from the data collection, where a wide area is often considered for the study. There are also constraints in realising larger systems on a laboratory scale. Such limitations can be overcome by numerical modelling.

Wu and Libchaber [10] carried out experimental investigations on passive beads in an active bacterial (*Escherichia Coli*) bath. They made use of soap film as a substrate upon which both these species are dispersed for interaction. Higher concentration of bacteria resulted in a fluctuated motion of beads where ballistic motion was observed for shorter distances and Brownian motion is detected at long time scales. Experimental investigations by Leptos et al. [11] on the dynamics of passive tracers in both dilute and dense bath of alga *Chlamydomonas Reinhardtii* revealed diffusive movement of the tracer particles. The probability distribution function for the same tracers showed a non-Gaussian (yet similar) form with an exponential tail and broadened base that grows along with swimmer concentration.

Numerical studies in the field have been carried out using both periodic and bounded domains, with most belonging to the former category. Periodic boundaries are usually used to study larger domains where a small unit of the larger domain is analysed. This helps reduce the computational cost and time considerably. Numerical simulations on active–passive particle mixture by Hinz et al. [12] using periodic boundaries demonstrated the emergence of three different phases—a disordered meso-turbulent phase, a polar flocking phase and a vortical phase. The manifestation of the vortical phase is sensitive to the domain size, whereas the other phases are indifferent. It is of particular importance that even a small number of active agents are capable of generating effective dynamics and associated patterns. Phase separation behaviour of an initially disordered mixture of monodisperse active–passive

system is reported in numerical investigations by Stenhammar et al. [5] with periodic boundary conditions. The phenomenon was observed with as low as a 1:6 active–passive particle ratio but at high activity. Their study suggested that by controlling the parameters like activity and active–passive particle ratio, one can transition the system between a homogeneous phase and phase separation. In another study by Dolai et al. [6], interaction between active–passive mixtures of different size ratios and different packing fractions were investigated with comparable volumes of active and passive particles. The results suggested the appearance of three distinct phases for the passive particles—a homogeneous phase, a clustered phase of small and large sizes, and a segregated phase where passive particle segregation is observed. Mixing behaviour of initially segregated binary system constituting only active particles has been investigated by Mahapatra and Mathew [13]. Here, both the particles are initially arranged in two separate boxes connected by a passage. In addition to self-propulsion force and interaction force, alignment and friction forces are also considered in the model. The system exhibits thermal, rotational and oscillatory phases at high packing fraction while exhibiting a predominantly rotational phase at lower packing fractions. The extent of mixing within the system is calculated using a mixing index, i.e., lower the mixing, higher the value of the index. Agrawal and Mahapatra [14] investigated the dynamics of an active-passive particle mixture with and without alignment force in a confined square boundary. Collective milling motion arises as a result of the alignment, whereas the absence of such a force results in a disordered phase. In most of the studies, where active particle systems or active–passive particle systems are investigated, the simulation is carried out in a 2D square domain. The dynamics of a binary mixture of self-propelling active particles and passive particles on a spherical surface is investigated by Ai et al. [15]. The particles are modelled as soft spheres and dynamics is governed by Langevin equations with holonomic constraint. Both rotational diffusion and polar alignment are considered, variation of which causes three distinct phases to occur—two segregated phases and one mixed phase.

From the literature, it is clear that several studies have been carried out to observe the dynamics of active–passive particle mixtures with cases varying from a single passive particle in a pool of active particles to passive particles with volume fractions comparable to active particles. Most of the investigations are in 2D with periodic boundary which not only reduces the complexity but also the computational time. With slight modifications, similar simulations carried out in a 2D surface can be realised over curved surfaces.

It is, however, interesting that there is a paucity of literature, where the active particles have been used to mix two or more different species of passive particles. The current chapter addresses this issue by demonstrating how a small amount of active mixer particles could be used to mix different passive species in a confined domain (which could also be realized under laboratory conditions).

3 Materials and Methods

3.1 Numerical Modelling

In the current work, we consider a monodisperse system of athermal particles arranged inside a 2D circular domain. The particle count is denoted by N_P for passive and N_A for active respectively. All the particles have the same radius (r). The domain radius (R) is chosen as $40r$. The wall of the bounded system constitutes of one layer of circular discs of the same size as that of interior particles. The packing fraction ($\emptyset$) is given by $\emptyset = Nr^2/R^2$, where N is the number of interior particles.

The dynamics of active particles is governed by the overdamped Langevin equations, consisting of a self-propulsion drive and an inter-particle repulsion drive (see Eqs. 1 and 2) [16].

$$\frac{\mathrm{d}\bar{r}_i}{\mathrm{d}t} = v\hat{n}_i + \mu \sum_j F_{ij} \tag{1}$$

$$\frac{\mathrm{d}\theta_i}{\mathrm{d}t} = \eta_i(t) \tag{2}$$

where $\bar{\boldsymbol{r}}_{\boldsymbol{i}}$ represents the position of the centre of particle i, v represents the self-propulsion speed of the active particles, in direction $\hat{n}_i = (\cos\theta_i, \sin\theta_i)$ μ and k are the mobility and the force constant, respectively. The repulsion force between the particles i and j (the surrounding particles of the particle i) acts when the particles overlap with each other and can be defined as, $F_{ij} = k\left(2r - d_{ij}\right)\hat{\boldsymbol{r}}_{\boldsymbol{ij}}$, where $d_{ij} = \left|\bar{\boldsymbol{r}}_{\boldsymbol{i}} - \bar{\boldsymbol{r}}_{\boldsymbol{j}}\right|$ and $\hat{\boldsymbol{r}}_{\boldsymbol{ij}} = \left(\bar{\boldsymbol{r}}_{\boldsymbol{i}} - \bar{\boldsymbol{r}}_{\boldsymbol{j}}\right)/d_{ij}$. The direction of the self-propulsion velocity depends on an angular Gaussian white noise η where $\left\langle \eta_i(t)\eta_i\left(t'\right)\right\rangle = 2D_r\delta_{ij}\delta\left(t - t'\right)$. D_r is coefficient of rotational diffusion.

The equation for passive particles differs from that of the active particles due to their inability to self-propel and is formulated in Eq. (3).

$$\frac{\mathrm{d}\bar{\boldsymbol{r}}_{\boldsymbol{i}}}{\mathrm{d}t} = \mu \sum_j F_{ij} \tag{3}$$

The parameters μ and k are assumed to have the same values for both active and passive particles. The wall particles are designed to be immobile barriers which confine the interior particles in the domain of interest by way of the repulsion drive. All the particles are assumed to be athermal, that is, the translational diffusion is considered to be negligible compared to the rotational diffusion [16]. To make self-propulsion velocity and time dimensionless, they are scaled by $r\mu k$ and $1/\mu k$ respectively. Scaled speed is represented by v_o and scaled time is denoted by τ.

The passive particles are segregated into two species. All the particles are initially arranged in a uniform random distribution such that one of the species of passive particles occupy the upper half of the domain and the other species occupy the lower

half. The active particles are then distributed in a uniform random sense within the entire circular domain. The initial orientations of the active particles are also uniformly randomized in the range $[0, 2\pi]$.

Passive particle packing fraction $\left(\emptyset_P = \pi \sum_{i=1}^{N_P} r_i^2 \Big/ \pi R^2\right)$, that is, the ratio of the area occupied by the passive particles (numbering N_P) to the total area of the domain is 0.6 and is maintained invariable across all the simulation cases. Simulations are carried out, altering the number of active particles by defining an active–passive particle fraction ($\Psi = N_A/N_P$). The value of Ψ is varied from 0.1 to 0.5 so that the maximum overall packing fraction ($\emptyset = \emptyset_A + \emptyset_P$) is not more than 0.9. Euler-Maruyama scheme is employed for numerical integration of Eqs. 1–3 with a timestep 10^{-2} s.

Figure 1 showcases a representative initial distribution of particles in the domain. The passive species are coloured blue and green, while the active particles are coloured red respectively.

The simulations are carried out till the system reaches a stable state, indicated by the saturation of a mixing parameter defined in the next subsection. The simulations are run using an in-house code written in Python *3.7* along with the JAX functionality for highly parallel GPU computations.

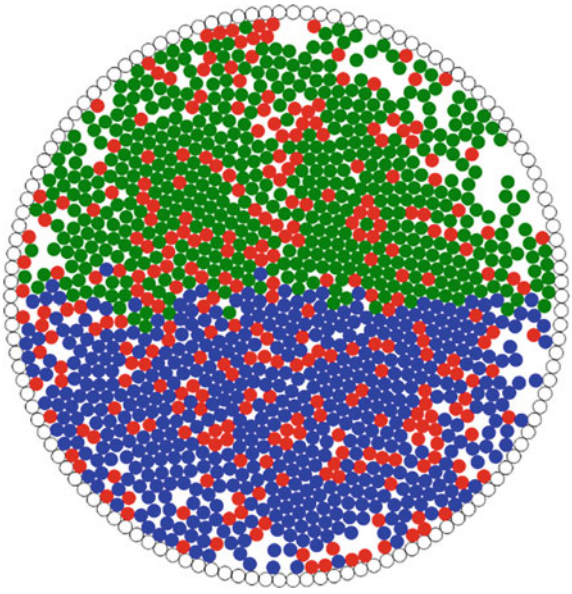

Fig. 1 Distribution of active and passive particles inside the circular domain; ($\Psi = 0.3$)

3.2 Mixing Parameter

Mixing index (β) quantifies the degree of mixing of the two passive species on the basis of the current and the initial positions of the particles. The calculation of the mixing index follows the weak sense mixing technique proposed by Doucet et al. [17], employing Principal Component Analysis (PCA) to compute the Eigen values of the position matrix, and used a priori by Mahapatra and Mathew [13]. We define the mixing using a mixing parameter, $\gamma = 1 - \frac{\beta(\tau)}{\beta_0}$, where $\beta(\tau)$ is the current mixing index and β_0 is the mixing index for the initial particle distribution without overlap. Higher values of γ represents a better mix.

3.3 Validation

The numerical model used in the current work has been validated against the results reported by Yang et al. [16] on the interactions among mono-dispersed self-propelling athermal disks in a confined square-shaped 2D space. For a range of parameters such as diffusion coefficient, self-propulsion velocity and overall packing fraction, they observed particle aggregation at the walls and quantified it using Gini coefficient (ζ). Gini coefficient is calculated by dividing the domain in to 'n' concentric squares of equal width and applying the equation $\zeta = \frac{1}{2n^2|\overline{\rho}|} \sum_i \sum_j \left|\rho_i - \rho_j\right|$, where ρ is the particle number density in the corresponding strip and $\overline{\rho}$ is the mean density. Higher the value of ζ (beyond 0.50), the system is wall aggregated where as a lower value represents homogeneous state. Using our numerical model with the parameter set and domain properties, the results are found to be in good agreement with those reported by Yang et al. [16] (Fig. 2). Two values of overall packing fraction are considered (0.720 and 0.831); the speed v_o is varied from 0.01 to 0.10 and the Gini coefficient is computed for each v_o after the system reaches a steady state. The results displayed are the average of five realisations that have been carried out for each parameter set and the curves seem to be in good agreement. The deviations at higher values of v_o can be attributed to the stochastic nature of the problem and the slight differences in the model/parameters used.

4 Results and Discussion

Preliminary simulations have been carried out to determine the parameter space for inducing mixing in segregated passive systems using active particles. Active particles with a low rotational diffusion coefficient D_r are found to have a tendency to aggregate at the walls instead of promoting mixing (Fig. 3; inset $D_r = 0.001$, $\tau = 2 \times 10^4$). Hence, a study is carried out to determine the optimum values of D_r to obtain maximum degree of mixing. The diffusion coefficient is varied in the

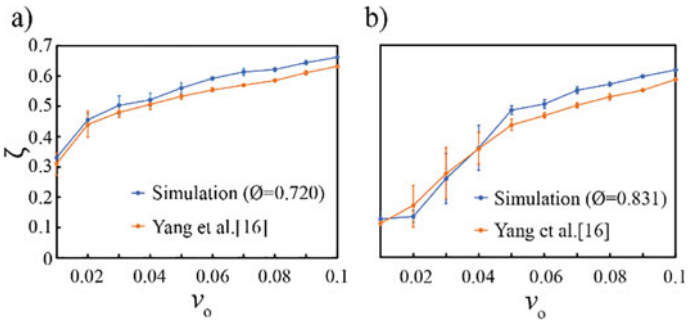

Fig. 2 Comparison of Gini coefficient ζ obtained from our simulation to that of Yang et al. [16] for overall packing fractions: **a** $\emptyset = 0.720$ and **b** $\emptyset = 0.830$; ($\mu k = 10\ \mathrm{s}^{-1},\ r = 1$)

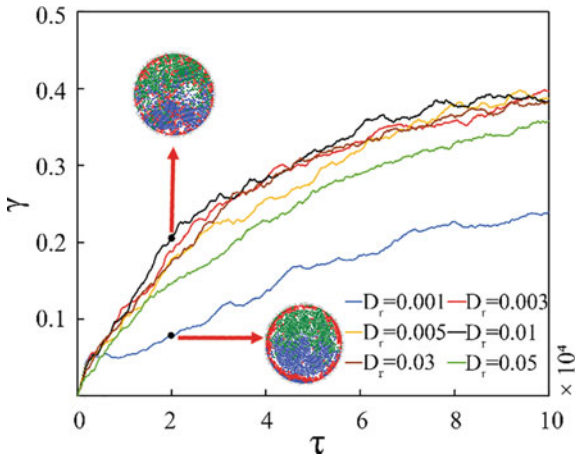

Fig. 3 Variation of mixing parameter γ with time τ for varying D_r; ($\Psi = 0.3$)

range of 0.001 to 0.05. With higher values of D_r, the active particles are observed to constantly agitate their passive counterparts. The system thus always maintains a dynamic state and the two species of passive particles undergo mixing across the domain. The quantification of this visually detected mixing phenomenon is done with the help of a mixing parameter, as discussed in the next subsection.

4.1 Effect of Rotational Diffusion on Mixing

The system is simulated for different values of D_r keeping the value of Ψ fixed at 0.3. The system is seen to have reached a steady state in around $\tau = 10^5$. The positional data of the passive particles is used to compute the mixing parameter γ throughout the time period of the simulation (see Fig. 3). For any value of D_r, γ is found to increase with the progression of time, as the active mixers keep agitating the

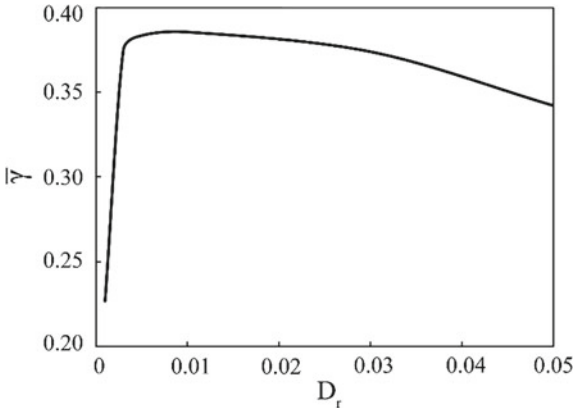

Fig. 4 Variation of time-averaged mixing parameter $\overline{\gamma}$ with rotational diffusion coefficient D_r; ($\Psi = 0.3$)

system. However, γ reaches a saturation at a value of around 0.4. There seems to be no further temporal change to the mixing parameter beyond this point. It should be noted, though, that at lower value of D_r (0.001), the value of γ is low in comparison to other cases. As D_r increases to 0.003, there is a sudden increase in γ establishing a better mix within the domain. Increasing the D_r further increases the value of γ albeit at a slower rate. To find out an optimum value of D_r for which γ is maximum, the simulation is further carried with higher values of D_r.

The average of γ in the range $\tau = 8 \times 10^4$ to 10^5 is plotted against D_r (Fig. 4). It can be noted that for lower values of D_r, an increase in the value of D_r increases γ rapidly. This is because the active particles, rather than aggregating at walls, move more vigorously in both rotational and translational manner. However, after reaching a maximum value at $D_r = 0.01$, a further increase in D_r decreases γ but gradually. This could be due to the fact that the active particles tend to undergo more of a local traverse (as they more often take larger turns) than a global one.

4.2 Effect of Active to Passive Particle Ratio on Mixing

The effect of concentration of active particles is studied by varying the active–passive particle fraction (Ψ) from 0.10 to 0.50 in steps of 0.10. For each case, the simulation is carried out until $\tau = 2.5 \times 10^5$. Longer run times ensure the occurrence of a steady state in the system. The rotational diffusion coefficient is set to the optimum value of $D_r = 0.01$. Figure 5 elucidates the occurrence of mixing reported by the mixing parameter γ through snapshots of the particle distribution within the domain at different instances of time. In the figure, four different time instances of the system are showcased corresponding to active–passive particle ratios Ψ:0.10, 0.30 and 0.50. When Ψ is 0.10, the active particle count is very low to cause sufficient agitation in the system for the mixing to take place. In addition, many of the active particles are concentrated adjacent to the wall. The gradual cross flow of the two passive

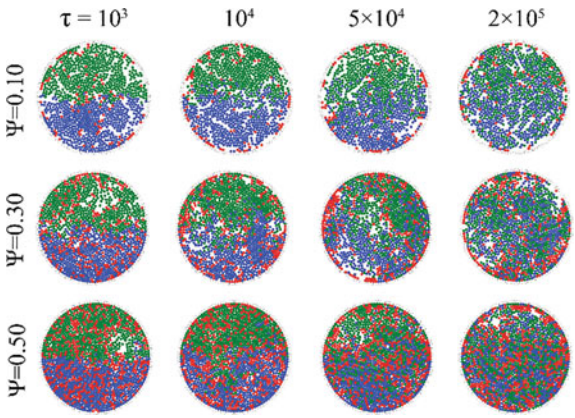

Fig. 5 Snapshots of the system for different active to passive particle ratios ψ at various time instances

species is also elucidated as the time progresses. At $\Psi = 0.30$, the aggregation of active particles near the wall is still evident, albeit to a lower extent. Mixing has improved as there are more active particles dispersed within the domain. Mixing at $\Psi = 0.50$ is comparable to that at 0.30, except the fact that we can see a more uniform distribution of active particles within the domain. In addition, the aggregation of active particles near the wall is less prominent. Ideally, this should further increase the mixing parameter, but a larger number of active particles has created a near-jammed state in the system which leads to local confinement of the active particles and subsequently the inability to move the passive particles.

The manifestation of activity-induced mixing in the domain can be visually confirmed in Fig. 5. To quantify the extent of mixing, the mixing parameter is established (see Sect. 3.2) and computed for the different values of active–passive particle fractions Ψ. The variation in the rate of mixing with the increase in Ψ, delineated in Fig. 6 corroborates the observations from Fig. 5. A striking feature of Fig. 6 is that all the curves (pertaining to different Ψ) tend to attain a similar value of γ (~0.40) at steady state. At a very low concentration of active particles ($\Psi = 0.10$), the curve is less steep which implies a longer time for the system to attain a steady mix. By increasing Ψ to 0.20, i.e., by doubling the number of active particles, mixing is achieved at a faster rate and steady state is achieved at a considerably lower time. Increasing the Ψ further to 0.30 helps achieving the same steady state γ at roughly half the time compared to $\Psi = 0.10$. Further increasing Ψ to 0.40 does not cause any significant change in γ or in the time taken to achieve steady-state mixing. Any further hike in the number of active particles proves to be detrimental to mixing as accentuated by the reduction in γ at $\Psi = 0.50$. The analysis of the rate of change of mixing parameter for the different active–passive particle fractions depicts a requirement of the number of active particles not exceeding 20% of the number of passive particles, in order to obtain brisk mixing.

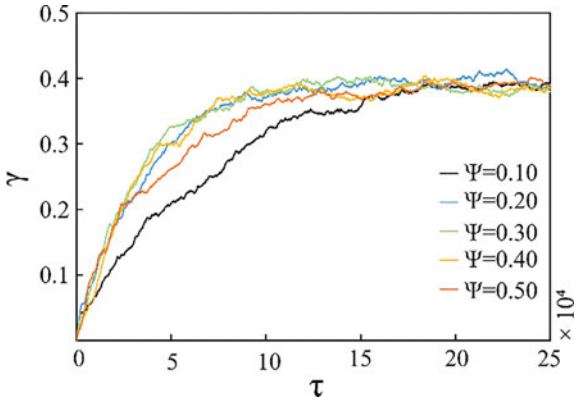

Fig. 6 Change in mixing parameter γ with time τ for varying Ψ; ($D_r = 0.01$)

5 Conclusions

The behaviour of an initially segregated binary system of passive particles is studied in the presence of a controlled number of active athermal mixers. The system constituting of the two passive species and the active mixers placed in a confined circular domain are modelled using a set of overdamped Langevin equations. At low values of rotational diffusion coefficient, the active mixers are found to aggregate along the wall, leading to little mixing of the passive species. For a certain value of passive packing fraction and active–passive particle fraction, it is found that there exists an optimum value of rotational diffusion coefficient for which mixing occurs most efficiently. The mixing of the two passive species is measured in terms of a mixing parameter based on the Eigen values of the position matrix at any time instant compared to that of the initial positions. In the base case considered ($\emptyset_P = 0.60$, $\Psi = 0.30$), the optimum value for D_r is obtained as 0.01. It is also observed that the concentration of active particles is a major factor affecting the rate of mixing. However, the extent of mixing in the system on reaching steady state (at large time scales) remains largely unaltered across different active particle concentrations. An important outcome from the current study is the number requirement of the active mixers for obtaining sufficient mixing at comparatively low time scales. It is noted that an active–passive particle fraction not exceeding 0.2 provides ample agitation to cause brisk mixing of the passive species. Due to the confined boundary conditions and the experimentally relatable parameter set, this study could find application in the case of artificial micro-robots to obtain rapid mixing among various living/artificial entities.

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Nomenclature

r	Particle radius [m]
R	Domain radius [m]
v_o	Non dimensional self-propulsion speed [–]
$\overline{\boldsymbol{r}}$	Position vector [–]
μ	Mobility [s/kg]
k	Force constant [N/m]
Ψ	Active-passive particle fraction [–]
D_r	Rotational diffusion coefficient [rad^2/s]
γ	Mixing parameter [–]
η	Gaussian white noise [–]
τ	Non dimensional time [–]

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