Topical: Developing Architected Materials for Controlling Fluid Flow and Interfaces

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Introduction

Reliable and predictable control of liquid and gas flow in space is a vital component of space missions. Critical aspects of water management for life support systems, fuel delivery in spacecraft engines, thermal management using heat pipes, and lab-on-a-chip diagnostics are all highly impacted by fluid behavior in the absence of gravity [1–3]. While admirable progress on these fronts has been made over the last decade, control of multiphase flow and interfaces remains a challenge.

Capillary effects in microgravity occur at much higher length scales that on Earth, which can be used to regulate fluid pathways and interfaces by controlling the structure and wetting properties of their containers. This approach of taking advantage of surface tension- riven flow can be much more energy-efficient than relying on acceleration or moving parts to ensure phase separation.

The last decade has seen the emergence of rapidly growing field focusing on the design of architected materials, typically ordered lattices of beam-based or wall-based unit cells tessellated in three dimensions. The expansion of high performance computing capabilities has allowed design optimization algorithms to produce complex non-intuitive designs. The fabrication of these complex structures has been enabled by advances in additive manufacturing technology. These methods can hence produce novel constructs that combine innate material properties with specifically designed architectures to achieve previously unobtainable combinations of structural, mechanical, thermal, optical and other functional properties [4–10].

To date, control over fluidic processes has been an underexplored space for this emerging area. However, recent notable studies have shown that architected materials can be designed to control fluid flow and placement, as week as fluid-fluid and fluid-solid interfaces in three dimensions [11–13]. The deterministic structure of these materials allows the development of predictive analytical and numerical modeling approaches to improve the fundamental understanding of static and dynamic gas-liquid-solid interfaces and surface tension-driven flow in three dimensions. Moreover, this fundamental understanding can be used to drive design optimization algorithms to produce optimal lightweight structures for fluidic control.

This paper presents an outlook on the use of multifunctional architected materials in space to enable new fluid management technologies, as well as the modeling and testing challenges inhibiting predictive design and optimization. We address design considerations for several example use cases and discuss the prospects of on-demand additive manufacturing in space.

Control of gas-liquid and liquid-liquid interfaces in microgravity

The dimensions at which liquids will experience capillary flow is often described by the capillary length (λ), a scaling factor that relates surface tension and the specific weight of the liquid. For water, the capillary length is approximately 3 mm on Earth and 6.68 mm on the moon. In microgravity, this characteristic length increases by several orders of magnitude. The dimensionless Bond number, which represents the ratio of gravitational and surface tension, relates the capillary length to the characteristic length of the system ($Bo = (L/\lambda)^2$). In microgravity, the Bond number becomes infinitesimally low and deriving meaning from its absolute values becomes difficult. However, early experiments aboard the ISS indicate that surface tension-driven liquid flow can still be controlled by managing the relative difference in characteristic lengths (e.g., the astronauts' coffee cup).

Architected materials provide a tremendous opportunity to take advantage of this phenomena, because they can be deterministically designed to have spatially varying structures and densities across length scales of several orders of magnitude (microns to tens of centimeters), and in three dimensions. Recent findings have shown that even small changes in the relative density of unit cells of architected lattices can drive preferential liquid flow in desired conduits (Fig. 1). However, it is imperative to understand what the impact and scale of these characteristic length differences at extremely low Bond numbers, where surface tension forces are so highly dominant. Hence, systematic experiments in microgravity are needed to get further insight into these effects and enable rational design of fluidic devices for space. In addition, the knowledge gained from these studies would benefit the understanding of capillary phenomena on Earth at comparable Bond numbers, i.e. extremely low length scales such as flow in nano-porous media, which can be difficult to characterize experimentally.

Similarly, architected materials of known structure can be utilized to understand characteristic time scales of surface tension driven processes and the stability of gas-liquid interfaces. On Earth, dynamic phenomena such as oscillations of gas-liquid interfaces occur on millisecond time scales [11]. The absence of gravity that gives way to pronounced surface tension effects could also play a role in the relative importance of inertial and surface tension forces. Architected materials can be designed to position and stabilize interfaces, as well as study the critical pressures required to break those interfaces. These findings would further facilitate the ability to handle bubble and droplet formation and phase separation.

Finally, the wetting properties of materials can be a key factor in controlling fluid flow via surface tension forces. The wetting behavior can be a function of both the material's intrinsic surface chemistry, as well as the structural topology of the surface on the micro- and nanoscale. Recent advances in additive manufacturing fabrication methods and an expanding materials palette could allow the creation of architected materials where combinations of these factors could be investigated and utilized.

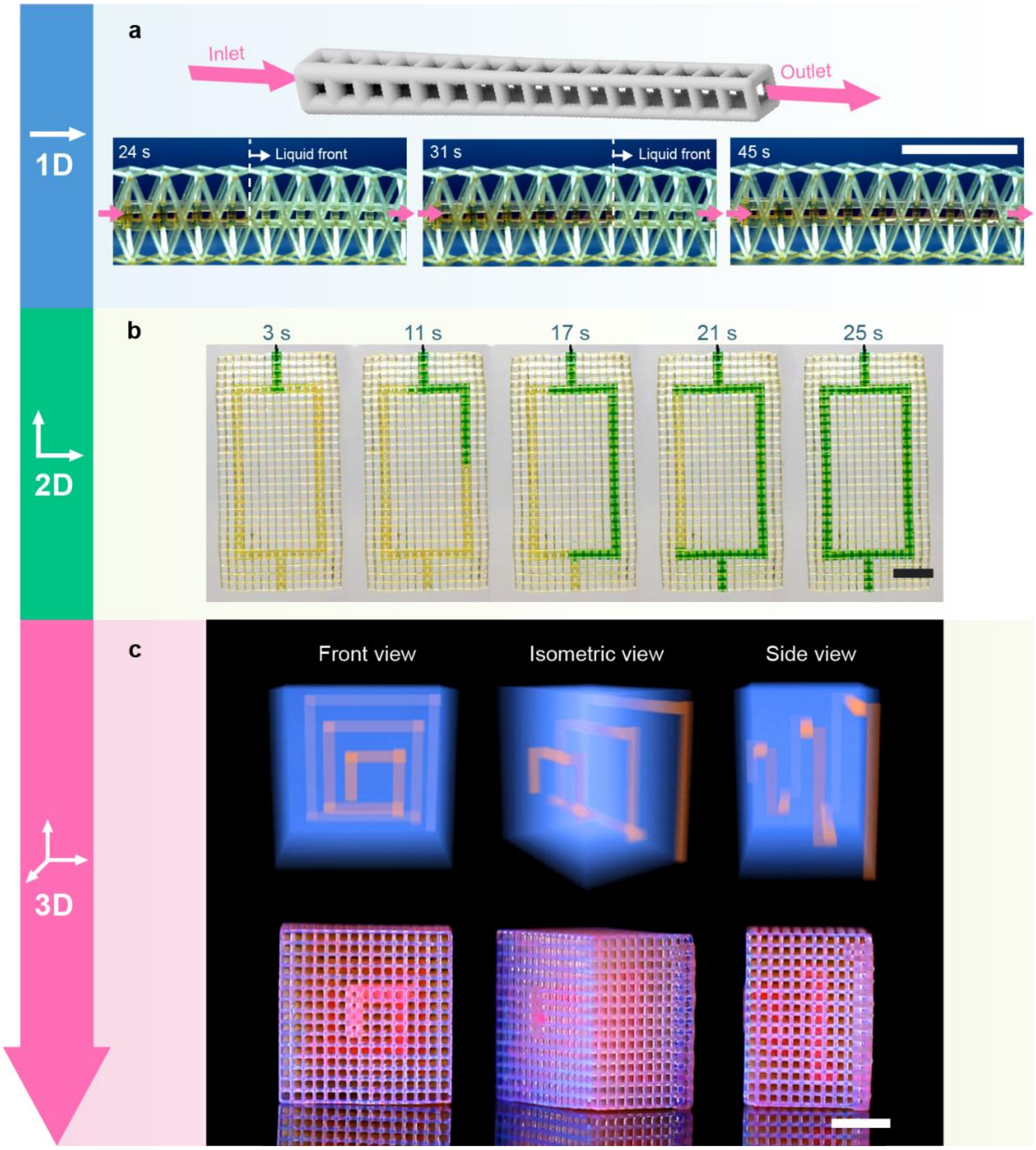

Fig. 1. Architected materials designed to control fluid flow and interfaces (adapted from Dudukovic et al., *Nature* 2021 [11]**). (a)** Single channel of simple cubic cells with a gradient in strut diameter, facilitating flow in the desired direction. **(b)** Selectively increasing the relative density in a desired pattern creates preferential liquid pathways through a lattice. **(c)** A spiral-like 3D liquid path achieved by controlling the local strut diameter.

Modeling of fluid behavior in architected materials and design optimization

The ability to deterministically design unit-cell based architectures enables the creation of ordered porous media. Modeling porous structures with repeating units of known geometry – rather than random, heterogeneous foams – can be simplified by describing a repeating subset of the structure or a single unit cell, rather than averaging across areas and volumes. This allows analytical modeling of capillary flow and steady-state interfaces. However, when studying nonsteady state dynamic phenomena, modeling multiphase flow can be computationally intensive due to solver limitations and moving mesh boundary challenges. Grid- or mesh-based numerical methods require small time step increments to converge, and can often require weeks to simulate processes on relevant timescales. Hence, the design of new architectures for controlling fluid flow could be made more efficient if the modeling of dynamic phenomena can be circumvented when possible, e.g. treating interfaces as steady-state while operating within analytically-derived pressure regimes that do not disrupt the interface. Finally, design optimization algorithms have been successfully used to produce optimized structure for mechanical, thermal, electrochemical etc. performance [14, 15]. Similar approaches can be used to design novel non-intuitive cell-based architectures for fluidic control. These efforts will require the development of forward physics models that capture the relevant boundary conditions, identifying target performance metrics, and incorporating manufacturing constraints.

Use case scenarios and design considerations

Recent demonstrations have shown the potential of architected materials to control fluids in a variety of processes. Architectures can be designed to direct flow of liquid sorbents for CO_2 capture with tunable gas-liquid interfaces, where interfacial area can be maximized across a volume based on surface tension-driven interactions. Transpiration cooling in heat pipes is another process that could be optimized by employing architected materials to control the transport of the condensed phase. Facilitation of phase separation or coalescence is another area where employing deterministically designed geometry based on fundamental understanding of fluids and interfaces can be beneficial. Finally, producing structured catalysts and packed beds for chemical or electrochemical reactors and fuel cells from architected materials introduces the potential for better control of multiphase interfaces for highly impactful processes.

On-demand fabrication of architected materials in microgravity

Architected materials can be designed to be lightweight (and in some cases collapsible) and can thus be well-suited for launch missions. However, the ability to manufacture parts on demand could allow rapid design iteration. Fabrication of complex structures such as microarchitected lattices and triply periodic minimal surfaces has been enabled by advances in various additive manufacturing (AM) technologies. In microgravity, extrusion-based 3D printing or powder-based fabrication processes such as selective laser sintering and binder jetting are difficult to carry out due to challenges in material handling. Light-based methods such as stereolithography operate by projecting a light pattern onto the surface of a photocurable polymer to solidify it. The process is repeated for each subsequent layer as the part is immersed into a fresh layer of liquid resin; thus, handling the liquid photopolymer resin can pose challenges in microgravity. In general, most layer-by-layer AM processes rely on gravity in some way (e.g., leveling of liquid layers, spreading of powder layers, adhesion of extruded layers, etc.) and require modifications to operate in space. However, recent developments in volumetric light-based additive manufacturing have enabled production of entire 3D objects within a liquid resin volume. Therefore, volumetric AM methods are less limited by the absence of gravity and hold promise for fabrication in space.

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This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE AC52-07NA27344.