RESEARCH

Application-Specific Computational Materials Design via Multiscale Modeling and the Inductive Design Exploration Method (IDEM)

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Received: 1 December 2016 / Accepted: 16 December 2016 / Published online: 22 March 2017
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Abstract The development of materials is a laborious, iterative, expensive, and intuitive process, often requiring decades to transition from early laboratory studies to commercial applications. This research seeks to address this issue by demonstrating a systematic process for linking process-structure-property-performance (PSPP) relations. We argue that the limitations on time for the *material development process* arise in large part due to lack of effective approaches for exploring the material design space that anticipates application requirements, objectives, and constraints. The *material design process* employed here utilizes hierarchical multiscale modeling, analytical models, and associated metamodels to construct a set of bottom-up deductive mappings, along with the inductive design exploration method (IDEM) to account for uncertainty in pursuing top-down inductive decision support problems that address application-specific design objectives. The demonstrated problem considers the simultaneous design of ultra-high-performance concrete material and a structural panel able to withstand a 1.5-MPa-ms reflected blast wave impulse. A set of PSPP mappings were constructed across micro-, meso-, and macro-length-scales using analytical expressions and a hierarchical multiscale finite element model at the single fiber,

multiple fiber, and structural length scales. The set of PSPP deductive mappings considered seven design variables—panel thickness, fiber pitch, ratio of water to cementitious materials, curing temperature, and volume fractions of fibers, cement, and silica fume—across four hierarchical levels. After the set of deductive PSPP mappings were constructed and validated, ranged sets of feasible values for each design variable were determined via IDEM. Starting with the highest and next-to-higher hierarchical levels as the output and input spaces, respectively, IDEM was implemented via application of three steps—discretization of input variables, projection of discretized sets of input variables with account of uncertainty to a range in the output space, and determination of which sets of discrete input values satisfy the output space requirement(s). By recursively applying these three steps, the PSPP relations were robustly searched for properties, structures, and processes that satisfy the performance requirement(s). The advantages of this approach are the identification of ranged sets of values of design variables and the ability to account for propagated uncertainty. By defining additional mass and cost objectives, the feasible input space was then searched to find the preferred combination of values of design variables that minimized mass and minimized cost while maintaining a robust material and structural design.

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Keywords Multiscale modeling · Inductive design exploration method (IDEM)

Introduction

Civilization and materials are inexorably linked, so much so that long time spans, such as the Stone Age and the Bronze Age, were named for the dominant material of the era. The connection between advances in civilization and advances in

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materials has been further cemented through the industrial revolution and the information age. The process of developing new materials historically was, and still vastly is, a laborious, iterative, and intuitive process characterized by four steps: (1) generate an idea for a new material; (2) process the new material via trial-and-error methods in a laboratory environment; (3) characterize the new material for physical, chemical, and thermal properties; and (4) repeat steps one through three as required until the desired properties are produced. After realization, the new material must find a path to commercial viability. Commercial viability is defined by three criteria: (1) the new material must deliver capability in an application; (2) the new material must be capable of being processed and manufactured; and (3) the new material must be economically viable at the volumes required for the chosen application. Even if a new class of materials is produced, the time to commercial viability is typically on the order of 10 to 20 years, with wide-scale acceptance in commercial applications requiring an additional 20 years or more [1].

Once a material is conceived, the *material development process* has four systemic problems or challenges [2]. First, the final material design is often determined by perturbing the initial material design through a sequence of experimental trials. Thus, the final material design depends upon the initial material design and the choice of experimental pathways to produce variants of the initial material design, not upon a systematic search within the entire parametric space considered of material process-structure-property-performance (PSPP) relations. Second, the time required to execute and characterize each experimental material design trial limits the rate at which new materials can be developed. Third, the expense to execute and characterize each experimental material design limits the number of characterizations performed. As a result of these latter two problems, the number of experimental design iterates is quite limited (e.g., two to three iterates [3]), and the flexibility to search large portions of the potential design space is limited. Moreover, properties are improved until the performance requirement threshold is met. Fourth, the *material development process* can only produce materials and material designs that are possible with current manufacturing technologies. Even though material selection approaches (e.g., Ashby [4]) facilitate new application designs with a palette of available materials, the fundamental problems associated with the material development process remain. We note that material certification for products and regulatory considerations can also add considerable time to the development cycle and must be considered at early stages.

The problems associated with the material development process are exacerbated by batch-processed materials and extreme loading conditions, such as blast, impact, and rapid thermal exposure. Specifically, the physical experiments for extreme loading conditions can be even more expensive and lengthy than those employed for quasi-static loading

conditions. To rapidly adapt to current and future extreme loading conditions, a more structured and comprehensive approach such as the *material design process* is needed.

The concept of addressing PSPP relations in the *material design process* stems from Olson [5], who clarified the simultaneous deductive and inductive paths through a material's PSPP relations. The deductive path seeks to form accurate cause-and-effect relations in a bottom-up manner through PSPP relations, whereas the inductive path searches in a top-down fashion for properties, microstructures, and processing steps that satisfy the overall performance goals of the material in a specific design application scenario.

To realize a *material design process*, the roles of numerical simulations and physical experiments in the *material development process* must be reevaluated. For example, the *material development process* has employed trial-and-error experiments to search a parametric design whereas numerical solutions have been employed to understand results of physical experiments (e.g., [5, 6]). In the envisioned *material design process*, computational simulations are employed along with experiments and analytical expressions, with uncertainty of each quantified and expressed, to form the bases for the mappings involved in the bottom-up PSPP relations. To facilitate rapid parametric design space exploration, to the extent possible, these mappings are cast in the form of surrogate models or metamodels as is common in the multidisciplinary design optimization [2].

The complicated and time-sensitive nature of designing real materials warrants construction of metamodels from multiple sources. For example, metamodels constructed from analytical expressions and empirical data are justified if the analytical and empirical mappings exist and are bounded within an acceptable level of uncertainty. For analytical or empirical mappings having unacceptable levels of uncertainty or for necessary yet non-existent mappings, metamodels constructed from empirically validated numerical simulations may be preferred. By constructing the PSPP mappings via various forms of metamodels, optimization-based inverse material design algorithms have been employed (e.g., [7, 8]). Instead of seeking optimal solutions for materials whose performance may drop off significantly due to small changes in the assumptions, Choi et al. [9] sought to determine robust material designs that are insensitive to variation or uncertainty in design variables and computational models or metamodels, via the inductive design exploration method (IDEM). Robust material design algorithms, such as IDEM, have demonstrated faster convergence than that of an optimization algorithm [10], the ability to determine ranged vectors of feasible input parameters which may significantly reduce design iterations [11], and be able to account for propagated uncertainty across successive length scales [11, 12].

The objective of the present work is to demonstrate an implementation of a robust *material design process* based on

IDEM for a practical and highly non-trivial (i.e., high uncertainty) problem. The example problem considered is the design of an ultra-high-performance concrete (UHPC) blast panel intended to survive a predefined reflected impulse of 1.5 MPa-ms while minimizing the total mass of the panel. It is envisioned that by implementing such a *material design process*, the time to commercialize new blast-resistant UHPC structures will be reduced substantially.

Ultra-High-Performance Concrete

UHPCs are cementitious granular composites composed of Portland cement, sand, quartz powder, silica-fume, high-range water reducing agents, fibers, and water. The high-range water-reducing agents allow water to cementitious material ratios, w/cm , to be less than 0.3 without affecting the workability of the UHPC slurry [13]. In comparison to normal strength concretes (NSCs), which are composed of Portland cement, aggregate, sand, and water with w/cm ratios between 0.4 and 0.7, UHPCs are denser and have a less porous microstructure. Accordingly, denser UHPC microstructures have resulted in improved mechanical and mass transport properties. For example, UHPCs typically have quasi-static unconfined compressive and tensile strengths greater than 150 and 9 MPa [14], respectively, whereas NSCs have quasi-static unconfined compressive strengths on the order of 10 to 40 MPa and quasi-static unconfined tensile strengths on the order of 1 to 4 MPa [15]. The improved mass transport properties are quantified by improved freeze-thaw performance [16] and reduced chloride ion transport [17].

The development and commercialization NSCs and UHPCs have followed typical material development processes, resulting in decades from the invention of each granular cementitious material to the wide-spread commercialization. For example, Fig. 1 shows the annual consumption of Portland cement—used here as a proxy for the consumption of NSC—as a function of year from 1824 to 2012 [18–21]. Thirty-five years after the invention of “modern” Portland cement in 1845, only 22,000 t, or less than 0.5 kg per person, of Portland cement were consumed in the USA. In contrast, 415 kg per person of Portland cement were consumed in 2005. The lack of improvement in the material development process is evident in the commercialization time required by UHPCs. In the 34 years between the invention of

UHPC in 1978 and 2012, only 18 UHPC bridges were constructed in North America.

Uncertainty Analysis and the Inductive Design Exploration Method

Like many practical materials design and development examples, design of UHPC is characterized by ubiquitous uncertainty in the PSPP relations. Processing of cementitious materials is well known for its uncertainty, and the same is true for hierarchical structure-property relations. Hence, we consider robust design methods to mitigate uncertainty in design exploration. At least three types of robustness—type I, type II, and type III—may be employed to minimize the effects of uncertainty on output responses. Type I robustness seeks to minimize the variation in output responses as a function of noise variables [22]. Type II robustness seeks the desired performance levels while minimizing variation caused by control factors [23]. Type III robustness seeks to determine the desired performance level while minimizing the effects of uncertainty in the response function [10]. In a simulation- and metamodel-based material design process, type III robustness is critical to account for uncertainty in the structure-property relations, whether based on experiments or computational simulations. Hence, the consideration of uncertainty for the levels of inputs and the responses of metamodels as performed in the present analysis focuses on robustness of design solutions.

Figure 2 presents a schematic of the IDEM, which was employed to determine robust solutions through a recursive and systematic three-step method that determined feasible values of input variables for a given performance requirement. Although Fig. 2 shows IDEM with three spaces and two variables in each space, IDEM may be generalized to m -spaces with each space having up to n -variables, where m and n are positive integers. These mappings or projections can be based on theoretical or computational models, experiments, or some combination. They may constitute process-structure or structure-property relations. Adjacent (input to output) spaces to be mapped can correspond to *process to structure*, *structure to property*, *property to performance*, or even sequential evolution of material structure with processing steps, for example. Hence, the number of spaces depends on the decomposition of the hierarchy in time and space of the material PSPP relations,

Fig. 1 US cement consumption from 1825 to 2012 highlighting 35- and 34-year time spans from the invention of improved cementitious materials

Fig. 2 Schematic of inductive design exploration method (IDEM) applied to a three-level hierarchical problem consisting of x-, y-, and z-spaces. The schematic is shown with two variables in each space (Color figure online)

as discussed in “Methods” section. Between any two adjacent spaces, IDEM was implemented via application of three steps:

1. Discretize input variables
2. Project discretized sets of input variables with account of uncertainty to a range in the output space
3. Determine which sets of discrete input values satisfy the output space requirement(s)

For example, consider the adjacent y- and z-spaces shown in step 1 of Fig. 2 as an input and output spaces, respectively. The input y-space consists of two variables, y_1 and y_2 , discretized to a finite set of values, or “input values,” which are shown as black dots in step 1. In step 2, each input value is projected to the output z-space via the function g . Note that the projection of each input value creates a range of possible results, as indicated by the yellow ellipse in the output z-space. This yellow ellipse encompasses results from non-unique mappings or mappings involving uncertainty, thereby having a range of possible outcomes. In step 3, the range of outputs in z-space from a single input value is compared to the z-space performance requirement. If the range of output is within the z-space performance requirement, the input value satisfies the performance requirement.

To determine which input values satisfy a given output performance requirement, IDEM employs a hyper-dimensional error margin index (*HDEMI*) [9]. The *HDEMI* of the i th output space variable is defined as

$$HDEMI_i = \begin{cases} \min \left[\frac{\|(\mathbf{mean} - \mathbf{B}_j)\mathbf{u}_i\|}{\|(\mathbf{mean} - \mathbf{B}_j^i)\mathbf{u}_i\|} \right], & \text{for } \mathbf{mean} \in \Omega \\ -1, & \text{for } \mathbf{mean} \notin \Omega \end{cases} \quad (1)$$

where i is the number of variables in the output space, j is the number discrete points on a boundary, $\mathbf{mean}$ is the output value without considering types I, II, or III uncertainty, $\mathbf{B}_j$ is the output performance requirement composed of j points, $\mathbf{B}_j^i$ is the output boundary of a single input value in the i th output direction, $\mathbf{u}_i$ is a unit vector of the i th variable, and Ω is the feasible output space defined by $\mathbf{B}_j$. Note that $\|(\mathbf{mean} - \mathbf{B}_j)\mathbf{u}_i\|$ is the absolute value of the distance between $\mathbf{mean}$ and the boundary of the projected input point in direction of the i th output variable. Similarly, $\|(\mathbf{mean} - \mathbf{B}_j^i)\mathbf{u}_i\|$ is the absolute value of the distance between $\mathbf{mean}$ and the boundary of the output space projected in the i th direction.

The boundary of the output range of a single point, $\mathbf{B}_j^i$, is determined by the type or types of robustness desired. Given the input space $\mathbf{y} = \{y_1, \dots, y_k, \dots, y_n\}$, the input value $\mathbf{y}_0 = \{y_{1,0}, \dots, y_{k,0}, \dots, y_{n,0}\}$ projects to the $\mathbf{mean}$ output value $\mathbf{z}_0 = g(\mathbf{y}_0)$, where g is a function relating $\mathbf{y}$ and $\mathbf{z}$. Type II robustness accounts for variations in the output defined by

$$\Delta z = \sum_{k=1}^n \left| \frac{\partial g}{\partial y_k} \right| \Delta y_k, \quad (2)$$

where n is the dimension of the input space, $\left| \frac{\partial g}{\partial y_k} \right|$ is the absolute value of the partial derivative of g with respect to y_k , and Δy_k is the expected variation of the k th input variable. Type III robustness assumes knowledge of the deviation of the response function g . Specifically, the upper and lower bounds of g are, respectively, defined as g_{upper} and g_{lower} [11]. These bounds are typically based on a pseudo-likelihood estimate for error in simulations or

experiments, for example. In a similar manner to Eq. 2, the variation of z_0 due to g_{upper} and g_{lower} are defined as

$$\begin{aligned}\Delta z_{\text{upper}} &= \sum_{k=1}^n \left| \frac{\partial g_{\text{upper}}}{\partial y_k} \right| \Delta y_k, \text{ and} \\ \Delta z_{\text{lower}} &= \sum_{k=1}^n \left| \frac{\partial g_{\text{lower}}}{\partial y_k} \right| \Delta y_k.\end{aligned}\quad (3)$$

The maximum and minimum boundaries of uncertainty accounting for type II and III robustness are then defined as

$$\begin{aligned}z_{\text{max}} &= \text{Max} \{ g(y_0) + \Delta z, g_{\text{lower}}(y_0) + \Delta z_{\text{lower}}, g_{\text{upper}}(y_0) + \Delta z_{\text{upper}} \}, \text{ and} \\ z_{\text{min}} &= \text{Max} \{ g(y_0) - \Delta z, g_{\text{lower}}(y_0) - \Delta z_{\text{lower}}, g_{\text{upper}}(y_0) - \Delta z_{\text{upper}} \}.\end{aligned}\quad (4)$$

Finally, the deviation from the nominal value z_0 is found by

$$\begin{aligned}\Delta Z_{\text{upper}} &= z_{\text{max}} - g(y_0) \text{ and} \\ \Delta Z_{\text{lower}} &= g(y_0) - z_{\text{min}}.\end{aligned}\quad (5)$$

Discrete input values with $HDEMI > 1$ indicate the feasible input space; discrete input values with $HDEMI < 1$ indicate the infeasible space. However, a clear boundary between the feasible and infeasible space remains to be defined.

The boundary between the feasible and infeasible input spaces was determined by determining input values such that $HDEMI = 1$, as shown in Fig. 3. For each input value with $HDEMI > 1$, the input space is searched for nearest neighbors that have $HDEMI < 1$. Should a pair of input values be found with $HDEMI$ values greater than and less than 1, the $HDEMI$ value is calculated for the midpoint input value between the two corresponding input values. Following the bisection method to determine roots of equations, new input values are selected until the $HDEMI$ of the boundary point is within an acceptable tolerance of $HDEMI = 1$. The boundary identification process continues until the boundary is identified for the entire input space.

For design problems containing more than two levels and corresponding spaces, which of course pertains to most practical problems of interest, the performance at the highest-level space is used to determine the feasible input space at the next-to-highest space. The calculated feasible input space, or more specifically the boundary of the feasible input space, is employed via a convex hull approximation to determine the output performance requirement at the next-finer scale. In this recursive manner, IDEM can be used for problems across multiple levels of the PSPP relations, including material structure hierarchy in length scale and hierarchy of PSPP relations

Fig. 3 Determination of the boundary of an input space for a two-dimensional input space consisting of feasible and infeasible input points based on $HDEMI = 1$ in the output space (Color figure online)

in time (e.g., curing vs shock loading). Figure 4 shows the flowchart of the IDEM algorithm for a single mapping as implemented in MATLAB® [24].

Across a single mapping, IDEM accounts for uncertainty in the values of a discretized input variable and uncertainty of the metamodel, labeled as the f response surface in Fig. 4, by projecting a range of output onto the output space. The uncertainty in the value of a discretized input variable can be determined if measurements or computed data are available or can be estimated using engineering judgment lacking such information. Uncertainties of the metamodels can be determined by determining upper and lower bounds for each metamodel, i.e., f_{upper} and f_{lower} , respectively, in Fig. 4, via comparison with empirical, numerical, or analytical data, as done so in this work, or via engineering judgment. Propagated uncertainty between mappings is accounted for via IDEM's reliance upon HDEMI to determine feasible domains at the next adjacent lower level of hierarchy.

Methods

The considered example problem seeks to simultaneously design hierarchical material structure and a 1625.6-mm tall by 863.6-mm wide UHPC panel of an unspecified, but uniform thickness. The performance requirement is that UHPC panel should survive (i.e., not completely fracture due to) a blast load with a 1.50-MPa-ms reflected impulse applied to the proximal face. The remainder of this section describes the analytical and numerical relations employed within the

Fig. 4 Flowchart of the IDEM algorithm for a single mapping as implemented in MATLAB®. Multiple hierarchical PSPP levels are implemented via iterative application of this flowchart

deductive path and estimated errors associated with each employed relation.

Process-Structure-Property-Performance Mappings

Prior to implementing IDEM, a set of PSPP mappings were defined via metamodels, which for the example problem were derived via analytical expressions, empirical data, and computational simulations. The ability to incorporate metamodels from varied sources is advantageous and permits analysis of realistic materials design problems such as the present case. The PSPP mappings shown in Fig. 5 define the relevant relations to estimate the blast response of a UHPC panel subject to blast loading. Starting with the left-most column in Fig. 5,

processing steps (e.g., Mix constituents, Curing) are identified by rectangles. Within each rectangle, the processing step is shown in bold font, non-considered variables are shown within parentheses, considered variables are shown in plain font, and symbols for the considered variables are shown in italics. The arrows indicate a temporal sequence. The remaining right-most three columns, labeled “Structure,” “Response,” and “Performance,” contain individual mappings which are identified via rectangles. Mappings within the Structure, Response, and Performance columns are vertically classified by the length scale at which the mapping occurs, e.g., macro-scale, meso-scale, and micro-scale, thus facilitating delineation of the PSPP mappings for a multiscale material such as UHPC. Within each rectangle, the name of the mapping is

Fig. 5 Process-structure-property-performance (PSPP) mappings for design of UHPC subject to blast loading (Color figure online)

identified by bold-font text (e.g., Single fiber pullout), the output variable(s) are identified by non-bold-font text, symbol(s) for output variable(s) are shown in italicized text, the numerical or analytical relation is shown graphically, and the length scale for the numerical model (if applicable) is shown in the lower left hand corner in italicized text.

Viewed from a deductive bottom-up framework, an output variable from a given mapping (e.g., pullout force, P , from the Single fiber pullout mapping) becomes an input variable to the next mapping (e.g., Tensile: fiber-reinforced matrix). In Fig. 5, deductive relations are graphically shown as a line connecting the right-most side of the output variable's mapping to the left-most side of the input variable's mapping. Although

deductive relations are generally read from the left to the right (e.g., fiber pitch, $pitch$, fiber length, L_f , and effective diameter of the fiber, d_f , were inputs to simulating the response of a single fiber pulled from a cementitious matrix), counter examples of the typical left-to-right reading of the cause-and-effect deductive relations exist (e.g., compressive strength, f_c , is an input to the single fiber pullout simulation). By discretizing the input and output spaces, IDEM is able to accommodate such interdependencies.

The remainder of this chapter provides details regarding the mappings shown in Fig. 5. In general, each section describes the model, validation, and the response surface, which was required for material design via IDEM.

Process-Structure Mappings

Mix Constituents and Curing Temperature to Porosity Model of Hydrated Ultra-High-Performance Concrete

A critical part of the design process is consideration of mix constituents and curing processes. The mapping between mix constituents and curing temperature, T_{cure} (deductive inputs), and the volume fraction of pores, V_{pore} , and mean pore radii, r_{pore} (deductive outputs), in the hardened cement paste was assumed to depend upon on the constituent volume fractions, constituent sizes, hydration of the cement paste, interfacial transition zone, and the curing procedure. To account for these dependencies, it was assumed that hydrated concrete consists of three phases: aggregate, bulk hardened cement paste (or bulk paste), and the interfacial transition zone (ITZ). The first phase, aggregates, consists of coarse and fine aggregates that were assumed to be non-reactive during the hydration process. Aggregates were characterized by their shape, specific gravity, and their distribution of sizes. Here, the volume fraction of aggregate, V_{agg} , is defined as volume of solids in the aggregate to the total volume of UHPC. The remaining volume was assumed to consist of bulk paste and ITZ.

The second phase, bulk paste, consists of porosity and the hydrated products of cement and water. Within bulk paste, the porosity is delineated into gel and capillary porosity. Adopting the definition used by Klobes et al. [25], gel porosity is defined as porosity with characteristic radii less than 25 nm, which represents the porosity within the calcium-silicate-hydrate (CSH) gel. Capillary porosity was defined as porosity with characteristic radii between 25 nm and 25 μm , representing the porosity between CSH gel structures.

The third phase of material, the ITZ, is a relatively porous region between the aggregate and the bulk paste. Although relatively thin with a typical thickness between 10 and 40 μm , ITZ can occupy up to 20 to 40% of the volume of the combined volume of bulk paste and ITZ in a normal strength concretes [21]. Similar to the bulk paste, the ITZ is delineated into gel and capillary porosity using the same radii-based definitions given above.

Figure 6 shows the set of assumed process-structure mappings used within the mix constituent and curing temperature to porosity (MCTP) model. Starting at the bottom of the process column, V_{cem} is the volume fraction of Portland cement, V_{agg} is the volume fraction of aggregate, V_{SF} is the volume fraction of silica fume, w/cm is the mass ratio of water to cementitious material, and T_{cure} is the curing temperature. In the structure column, V_{ITZ} and V_{paste} are the volume fractions of ITZ and bulk paste, respectively. The total volume fraction of pores, V_{pore} , is delineated into gel porosity within the bulk paste, $V_{\text{gel, paste}}$, capillary porosity within the bulk paste, $V_{\text{cap, paste}}$, gel porosity within ITZ, $V_{\text{gel, ITZ}}$, and capillary porosity within the ITZ, $V_{\text{cap, ITZ}}$, each with their own respective

characteristic radii, denoted by r with a respective subscript. Equations shown for bulk hydrated cement paste are from the well-established Powers hydration model [21] and empirical observations of reduced porosity at elevated curing temperatures [26, 27]. Equations shown for the interfacial transition zone account for the volume fraction of ITZ [28], size distribution and packing of aggregate [29], the hydration process via Powers hydration model [21], and empirical observations that the maximum porosity of the ITZ was two to three times that of the bulk cement paste [30]. The mean pore radius, r_{pore} , is a linear combination of the delineated pore radii and their respective volume fractions. Further details of the model and an example calculation are available in Ellis [24].

Results of the MCTP model are compared to empirical mercury intrusion porosimetry (MIP) data for NSC and HSC cured at room temperature and a UHPC cured at 250 °C in Table 1. MCTP material constants included composition and maximum aggregate size [25]; mean particle diameters and specific gravities for Portland cement, fly ash, silica fume, and quartz powder [21, 31]; and particle packing factors [29].

For the NSC, HSC, and UHPC samples, the MCTP model estimated V_{pore} values within 7% of those measured by Klobes et al. [25]. In addition, the MCTP model estimated similar distributions of pore sizes as the values reported by Klobes et al. [25] for the NSC and UHPC samples considered. However, the partitioning of porosity within the HSC sample was qualitatively incorrect: the MCTP model estimated a majority of porosity within the gel pores, whereas measurements indicated the opposite. One possible explanation for the discrepancy was the assumed 25-nm demarcation radius between gel and capillary porosity. This possible explanation is supported by the pronounced peak in frequency of pore size distribution near the 25-nm radius [25], which happens to be the demarcation radius between gel and capillary pores. Thus, small experimental measurement errors or small errors within the MCTP model could alter the gel-capillary partitioning of porosity.

The average pore radii, r_{pore} , estimated by the MCTP model shown in comparison to experimentally measured average pore radii in Fig. 7. In Fig. 7, the solid black line represents a one-to-one correlation and the two dashed gray lines represent $\pm 10\%$ deviation from a one-to-one correlation.

The aggregate size distribution for the remainder of this paper was assumed to be as follows: (1) 11% volume fraction of V_{agg} had a diameter of 0.075mm, (2) 18% of the volume fraction of V_{agg} had a diameter of 0.15mm, (3) 24% volume fraction of V_{agg} had a diameter of 0.30mm, (4) 29% volume fraction of V_{agg} had a diameter of 0.60mm and (5) 18% volume fraction of V_{agg} had a diameter of 1.18mm, which is in general agreement with the 2-mm maximum aggregate size reported for UHPC by Klobes et al. [25]. The specific gravity and packing factors for aggregates were assumed to be 2.7 and

Fig. 6 Process-structure (PS) relations used to determine volume fraction of porosity, V_{pore} , and the mean pore radius, r_{pore}

Table 1 Comparison of porosity volume fractions from MCTP model and MIP experimental data of Klobes et al.

Concrete	Normal-strength concrete (NSC)		High-strength concrete (HSC)		Ultra-high-performance concrete (UHPC)	
	MCTP model	Klobes et al. [25]	MCTP model	Klobes et al. [25]	MCTP model	Klobes et al. [25]
Parameter						
V_{agg}	0.677	0.677	0.619	0.619	0.527	0.527
V_{ITZ}	0.101		0.101		—	
$V_{gel, ITZ}$	0.020		0.018		—	
$V_{cap, ITZ}$	0.053		0.024		—	
α_{actual}	1.00		0.524		0.548	
V_{paste}	0.222		0.280		0.473	
$V_{gel, paste}$	0.044		0.049		0.064	
$V_{cap, paste}$	0.058		0.016		0.028	
Results						
V_{pore}	0.175	0.169	0.107	0.114	0.085	0.088
$V_{gel, pore}$	0.064	0.055	0.067	0.036	0.064	0.061
$V_{cap, pore}$	0.111	0.112	0.040	0.076	0.021	0.026

Source: [25]

Fig. 7 Comparison of average pore radii, r_{pore} , measured experimentally via mercury intrusion porosimetry (MIP) on the horizontal axis [25] and estimated via MCTP model on the vertical axis. The solid black line represents a one-to-one relation, and the dashed gray lines above and below the black line represent errors of $\pm 10\%$

0.56, respectively [31, 32]. The fineness modulus of the assumed aggregate was 3.25 [21]. The MCTP model was employed to estimate volume fraction of pores, V_{pore} , and average pore radii, r_{pore} , for a 540-data-point parametric space encompassing $T_{\text{cure}} = [20, 90]$ (°C), $V_{\text{cem}} = [0.09: 0.03: 0.21]$ (), $V_{\text{SF}} = [0.01: 0.01: 0.06]$ (), and $w/cm = [0.18: 0.02: 0.34]$ (). In the preceding sentence, numerical values separated by a comma are individual numerical values; numerical values separated by colons state the minimum value (first number), the step or increment size (the middle number), and the maximum value (third number). The unit of measure is given within the parentheses immediately following the bracket. Results of the 540 different simulations were then fit to two regression models:

$$V_{\text{pore}}(w/cm, V_{\text{cem}}, V_{\text{SF}}) = -0.00398 - 0.000167T_{\text{cure}} + 0.201V_{\text{cem}} + 0.193V_{\text{SF}} + 0.298w/cm - 0.000761T_{\text{cure}}V_{\text{cem}} - 0.000735T_{\text{cure}}V_{\text{SF}} - 0.00198T_{\text{cure}}w/cm - 0.315(V_{\text{cem}})^2 - 0.558V_{\text{cem}}V_{\text{SF}} + 1.37V_{\text{cem}}w/cm + 1.08V_{\text{SF}}w/cm - 0.165(w/cm)^2, \quad (6)$$

Fig. 8 Comparison of V_{pore} estimated via regression (i.e., Eq. (6)) and V_{pore} estimated by the MCTP model. The solid black line represents a one-to-one relation, and the dashed gray lines above and below the black line represent errors of $\pm 10\%$

Fig. 9 Comparison of r_{pore} estimated via regression (i.e., Eq. (7)) and r_{pore} estimated by the MCTP model. The solid black line represents a one-to-one relation, and the dashed gray lines above and below the black line represent errors of $\pm 15\%$

and

$$r_{\text{pore}}(w/cm, V_{\text{cem}}, V_{\text{SF}}) = 70.9 - 0.76T_{\text{cure}} - 71.5V_{\text{cem}} - 91.1V_{\text{SF}} - 16.8w/cm + 1.10T_{\text{cure}}V_{\text{cem}} + 1.33T_{\text{cure}}V_{\text{SF}} + 0.307T_{\text{cure}}w/cm - 31.9(V_{\text{cem}})^2 - 309V_{\text{cem}}V_{\text{SF}} - 65.2V_{\text{cem}}w/cm - 64.5(V_{\text{SF}})^2 - 78.3V_{\text{SF}}w/cm. \quad (7)$$

Figure 8 compares V_{pore} as estimated by the regression model in Eq. (6) and the estimation of V_{pore} by the MCTP model. Within the relevant parametric space considered, the regression model predicted the result of the MCTP model within 10%.

Figure 9 compares r_{pore} as predicted by the regression model in Eq. (7) and the prediction of r_{pore} by the MCTP model. The regression model predicts the result of the MCTP model within 15% except for $r_{\text{pore}} \leq 3$. In Fig. 9, there is a large gap in data for r_{pore} values between 10 and 33 nm. This gap is due to the substantial decrease in r_{pore} caused by curing at 90 °C.

Mix Constituents to Single Fiber

The mapping between the unconfined compressive strength of the cementitious matrix, fiber length, fiber pitch (i.e., length per one revolution for a helically twisted fiber about the fiber's axis), and fiber cross-sectional shape (deductive inputs) and the quasi-static pullout force-end slip relations (deductive outputs) were estimated via a 3D finite element (FE) model at the single fiber length scale evaluated via Abaqus/Explicit v6.10 [33]. Although a brief description is given below, Ellis et al. [5] provides a full description of the FE model at the single fiber length scale.

Figure 10 shows a sample instantiation of the FE model at the single fiber length scale, consisting of cementitious matrix (gray), fiber (green), and a 50- μm -thick ITZ (red) located between the fiber and the matrix. The lateral and back faces of the matrix (labeled 2–5 and 6 within the yellow rectangles,

Fig. 10 Finite element model at the single fiber length scale (Color figure online)

respectively) were fixed; the front face of the matrix (labeled 1 within the yellow rectangle) was free. The simulated fiber was placed within the matrix-ITZ to the fiber embedded length, L_e , displaced in the positive x_3 direction from the free end of the fiber, and slipped at the ITZ-fiber interface (i.e., relative motion between nodes of the fiber and nodes of the ITZ was allowed). The model at the single fiber length scale was employed to determine the pullout force-end slip relations of the fiber, where pullout force was defined as the total traction in the positive x_3 direction on the x_3 face of the fiber, and end slip was defined as the displacement in the x_3 direction of the x_3 face of the fiber with the reference position taken from the reference configuration (cf. Fig. 10).

All fibers were assumed to have triangular cross sections and 0.5-mm equivalent diameter, d_f . Here, equivalent diameter is defined as the diameter of the circle having the same cross-sectional area as the triangle, i.e., $d_f = 2\sqrt{A_f/\pi}$, where A_f is the cross-sectional area of the fiber. The model also assumed perfect geometric contact and slipping could only occur at the fiber-ITZ interface.

The matrix and ITZ were modeled via a pressure sensitive and strain-rate insensitive extended Drucker-Prager constitutive relation included within Abaqus v6.10 [33]. The fiber was modeled assuming a nonlinear isotropic-kinematic hardening constitutive relation included with Abaqus v6.10. The fiber stiffness and Poisson ratio were assumed to be 190-GPa and 0.33, respectively. A rate-independent, isotropic Coulomb friction model accounted for frictional effects at the fiber-ITZ interface. Based upon a 0.47 mean coefficient of friction for steel-concrete interfaces [34], a pressure-independent 0.45 coefficient of friction was assumed for steel-concrete interfaces. Accordingly, the model accounted for dissipated energy

due to granular flow of the ITZ and matrix, plastic work in the fiber, and frictional dissipation at the fiber-ITZ interface.

Calibration and Validation The remaining material parameters were calibrated using experimental results from Sujivorakul [35]. For example, material parameters for the fiber's nonlinear isotropic-kinematic hardening model were calibrated to experimental quasi-static, monotonically loaded tensile specimen data reported by Sujivorakul [35]. Further, the unconfined compressive strength of the matrix was assumed to match the 44 MPa reported by Sujivorakul [35]. A comparison of FE estimated and experimentally measured pullout force-end slip data for 12.7-mm embedded length fibers with 0.5-mm equivalent diameter triangular cross sections and 12.7- and 38.1-mm pitches is shown in Fig. 11.

Fig. 11 Validation curves for 0.5 equivalent diameters triangular fibers with initial pitches of 12.7 (red) and 38.1 (blue) mm. Experimental data of Sujivorakul [35] are shown as thick solid lines, and data from the FE model at the single fiber length scale are shown as thin dashed lines (Color figure online)

Considerations for Arbitrary Fiber Embedded Length

Calculations at the single fiber length scale were resource intensive, requiring up to 300 h on 40 AMD 2350QC processing cores to compute a single instantiation [5]. This relatively long computation time combined with the infinite number of possible fiber embedded lengths at the multiple fiber length scale presents a problem: it is intractable to calculate all possible pullout force-end slip responses required at the multiple fiber length scale.

As a solution to this problem, the pullout force, P , as a function of end slip, Δ , was calculated for each combination of fiber and matrix parameters of interest using the maximum fiber embedded length, $L_{e, \max} = L_{\text{fiber}}/2$, where L_{fiber} is the fiber length. An offset end slip, defined as $\Delta_{\text{offset}} = L_{e, \max} - L_e$, was then added to the actual end slip Δ of fibers with $L_e < L_{e, \max}$. The pullout force as a function of an arbitrary embedded length L_e and end slip Δ was then assumed to be equal to the pullout force at $L_{e, \max}$ and the combined end slip $\Delta + \Delta_{\text{offset}}$, i.e.,

$$P(L_e, \Delta) \approx P(L_{e, \max}, \Delta + \Delta_{\text{offset}}). \quad (8)$$

Figure 12 shows pullout force-end slip data from numerical simulations for a 12.7-mm pitch fiber embedded 2.5, 5.0, 7.5, 10.0, and 12.5 mm deep into a matrix. The matrix strengths are 44, 84, and 200 MPa for Figs. 12a–c, respectively. In each plot, data for the 12.5-mm embedded fiber and 2.5-mm embedded fiber

are shaded dark and light blue, respectively. Data at intermediate fiber embedded lengths are shaded in colors graded between dark and light blue. By plotting the pullout forces as a function of the combined end slip, the validity of Eq. (8) can be assessed. Although the pullout force-end slip data for $f_c = 44$ MPa do not overlay well for $L_e = 2.5$ and 5.0 mm, the pullout force-end slip data for $f_c = 84$ and $f_c = 120$ MPa overlay and are of greater interest for UHPCs.

Mix Constituents to Multiple Fibers

Individual fibers were assumed to be randomly placed and oriented within the UHPC microstructure with a fiber volume fraction defined by the mix constituents. It was further assumed that individual fibers did not undergo mechanical deformation during the mixing process; thus, the fiber length, cross section, effective diameter, morphology, and initial curvature were constant. Possible clumping, introduction of porosity due to clumping, and fiber orientation from wall effects were not considered. A 25-mm fiber length, 0.5-mm effective diameter, triangular cross section, 190-GPa fiber stiffness, 0.33 Poisson ratio, and material properties calibrated to experimental data of Sujivorakul [35] were assumed.

Fig. 12 Pullout force as a function of the addition of end slip and offset end slip for fibers with uniform 12.7-mm pitch for $2.5 \leq L_e \leq 12.5$ mm embedded within **a** $f_c = 44$ MPa, **b** $f_c = 84$ MPa, and **c** $f_c = 200$ MPa matrices (Color figure online)

Fig. 13 Sample instantiation of the rigid body-spring model (RBSM) at the multiple fiber length scale with $V_{\text{fiber}} = 1\%$, 25-mm fiber length, and 0.5-mm fiber diameter (Color figure online)

Structure-Property Mappings

Mapping Between Single Fiber Pullout, Multiple Fibers, Tensile Strength of the Matrix, and the Tensile Properties of a Fiber-Reinforced Matrix

The mapping between the single fiber pullout, multiple fibers, and tensile strength of the matrix (deductive inputs) and quasi-static maximum tensile strength and dissipated energy density of the fiber-reinforced matrix (deductive output) was defined via a rigid body-spring model (RBSM) at the multiple-fiber length scale and was based upon Bolander and Saito [36]. As shown in Fig. 13, the RBSM model consisted of two rigid elements, labeled 1 and 2, and desired volume fraction of fibers independently placed at pseudo-random locations and orientations within the two rigid elements. Note that fibers not crossing the $x_1 = 0$ plane were omitted from Fig. 13 for clarity.

Loading consisted of translating rigid element 2 in the positive x_1 direction while rigid element 1 was held stationary. Prior to cracking at the $x_1 = 0$ plane, the pre-cracking tensile stiffness was determined via a rule of mixtures approach, i.e.,

$$E_c = (1 - V_{\text{fiber}})E_m + \eta_l \eta_\theta V_{\text{fiber}} E_f, \quad (9)$$

where E_c is the elastic stiffness of the two-phase composite, V_{fiber} is the volume fraction of fibers, E_m is the elastic stiffness of the matrix, η_l is a parameter accounting for fiber embedded length defined as $\eta_l = 1 - \frac{\tanh(\beta L_{\text{fiber}}/2)}{\beta L_{\text{fiber}}/2}$, β is a parameter defined as $\beta = \sqrt{\frac{2G_m}{E_f r^2 \ln(R/r)}}$, G_m is the shear modulus of the matrix, E_f is the elastic stiffness of the fiber, r is the radius of the fiber, R is the mean radius of the matrix around one fiber, L_{fiber} is the total length of the fiber, η_θ is a parameter associated with orientation of fiber defined as $\eta_\theta = \frac{1}{N_f} \sum_{i=1}^{N_f} \cos^4 \theta_i$, N_f is the total number of fibers that cross the crack plane, and θ_i is the inclination angle of the i th fiber between the fiber's direction and that of the direction of displacement (i.e., x_1). At a displacement of $L_{\text{matrix}} \varepsilon_{\text{mu}}/2$,

the pre-cracking strength is $f_{t, \text{pre}} = E_c \varepsilon_{\text{mu}}$, where ε_{mu} is the fracture strain of the matrix without fibers.

After cracking at the $x_1 = 0$ plane, the RBSM assumed that the entire load was carried by the fibers [36]. This assumption is supported by empirical observations from blast testing of UHPC panels, which resulted in fracture surfaces having exposed fibers, very little debris, and relatively smooth and straight fracture surfaces [37]. Other dissipation mechanisms, such as comminution or frictional sliding, would have resulted in bent fibers at the fracture surface. Consequently, the evolution of tensile strength, $f_t(\delta)$, was calculated by summing the pullout resistance of each fiber bridging the crack, i.e., $f_t(\delta) = \sum_{i=1}^N f_{i\theta}(L_e, \delta)$, where $f_{i\theta}$ is the pullout of the i th fiber accounting for the inclination angle θ and L_e is the minimum embedded length in a Euclidian sense. In accordance with Li et al. [38], who determined effects of 0° to 60° inclination angles on straight, smooth fibers, $f_{i\theta}$ was assumed to be

$$f_{i\theta}(L_e, \delta) = \begin{cases} f_i(L_e, \delta) / \cos(\theta_i) & \text{for } -45^\circ \leq \theta_i \leq 45^\circ \\ f_i(L_e, \delta) / \cos(45^\circ) & \text{for } |\theta_i| \geq 45^\circ \end{cases} \quad (10)$$

By projecting pullout force-end slip relations on stochastically located and orientated fibers at the intermediate length scale, the RBSM model homogenized quasi-static traction-separation relations at a crack plane. The RBSM model was employed to determine the quasi-static tensile responses at the multiple fiber length scale of straight, smooth fibers, which were then employed to estimate responses of a UHPC panel to blast loading [39]. In accordance with experimental data reported by Sujivorakul [35], pullout force-end slip relations for fiber-containing morphology, i.e., polygonal cross sections twisted along the fiber length, were assumed to be zero for the final 20% of $L_{\text{fiber}}/2$.

Response Surfaces The RBSM was employed to calculate the quasi-static maximum tensile strength, T° , and dissipated energy density, G , for a 168-data-point parametric space encompassing $V_{\text{fiber}} = [0.5: 0.5: 2.0]$ (%), pitch = [6: 6: 36] (mm), and $f_t = [5.00: 1.07: 11.40]$ (MPa). Results of 100 instantiations were averaged to calculate a maximum tensile strength and dissipated energy density, as shown in Figs. 14 and 16, respectively. At $V_{\text{fiber}} = 0.5\%$, the maximum tensile strength of the fiber reinforced composite is dominated by increases in the matrix tensile strength, as indicated by the vertically-delineated iso-levels in Fig. 14a. However, for $V_{\text{fiber}} = 2\%$, the maximum pullout force of fibers of different pitch dominates the maximum tensile strength response as indicated by horizontal iso-levels in Fig. 14d.

The 168 data points used to generate the contour plots in Fig. 14 were fit to a rule of mixtures form, i.e.,

Fig. 14 Maximum tensile strength, T^o , as a function of fiber volume fractions between 0.5 and 2%, fiber pitch, and non-reinforced matrix tensile strength. All fibers had a 0.5-mm equivalent diameter and 25-mm length (Color figure online)

$$T^o = 3.47 + 0.569(1 - V_{\text{fiber}})f_i + 4830 \langle V_{\text{fiber}} - 0.00866 \rangle \text{pitch}^{-0.937}, \quad (11)$$

where $\langle \rangle$ are McCauley brackets signifying $\langle x \rangle = \frac{1}{2}(x + |x|)$, and 3.47, 0.569, 4830, 0.00866, and -0.937 are fitting parameters. The correlation between the data calculated by the multifiber length scale and the regression are shown in Fig. 15. The solid black line represents the regression shown in Eq. (11), and the dashed gray lines above and below the black line represent errors of $\pm 25\%$.

Fig. 15 Comparison of maximum tensile strength, T^o , as calculated by the model at the multiple fiber length scale (MFLS) and regression. The solid black line represents a one-to-one relation, and the dashed gray lines above and below the black line represent errors of $\pm 25\%$

Figure 16 shows the dissipated energy density as a function of fiber volume fractions between 0.5 and 2%, fiber pitch between 6 and 36 mm, and the non-reinforced matrix tensile strength between 5 and 11.4 MPa. The brittle nature of the matrix caused the dissipated energy density to be highly dependent upon the fiber volume fraction and pitch of the fiber. In Fig. 16, this behavior can be observed by the horizontal iso-levels of dissipated energy density, which increase with increasing fiber volume fraction. For comparison, the dissipated energy density for a fiber reinforced matrix having 200-MPa unconfined compressive strength and $V_{\text{fiber}} = 2\%$ of 0.185-mm diameter by 14-m long straight smooth fibers is 13.5 kJ/m², which is approximately one third that of a similar matrix with triangular cross section fibers with a 36-mm pitch.

The 168 data points used to generate the contour plots shown in Fig. 16 were fit to the regression

$$G = 0.166 + 4320 V_{\text{fiber}} - 62.4 V_{\text{fiber}} \text{pitch}, \quad (12)$$

where V_{fiber} is specified in decimal form, i.e., $0.005 \leq V_{\text{fiber}} \leq 0.02$, and pitch is specified in mm. Figure 17 compares G as calculated by the model at the multiple fiber length scale (MFLS) to G as calculated by the linear regression in Eq. (12). The solid black line represents a one-to-one correlation, and the dashed gray lines above and below the black line represent errors of $\pm 10\%$.

Fig. 16 Dissipated energy densities, G , as functions of fiber volume fractions between 0.5 and 2%, fiber pitch, and non-reinforced matrix tensile strengths. All fibers had a 0.5-mm equivalent diameter and 25-mm length (Color figure online)

Mapping Between Porosity and Compressive Strength

The mapping between porosity and compressive strength has been studied extensively. Powers [40] measured the volume fraction of porosity, V_{pore} , and the unconfined compressive strength, f_c , of cement pastes over the range $27 \leq f_c \leq 117$ MPa. The data were used to determine the empirical relation $f_c = 234(1 - V_{\text{pore}})^3$, where 234 is a constant representing the intrinsic strength of porosity-free cement paste and f_c is expressed in terms of MPa. Later, Odler and

Rößler [41] measured the distribution of pore radii within cement pastes over the range $4 \leq f_c \leq 112$ MPa that had been cured at temperatures between 25 and 100 °C. They fit their experimental data to the linear relation

$$f_c = c_0 + c_1 V_{\text{pore} < 10} + c_2 V_{10 < \text{pore} < 100} + c_3 V_{\text{pore} > 100}, \quad (13)$$

where c_0 , c_1 , c_2 , and c_3 are empirically determined parameters, and $V_{\text{pore} < 10}$, $V_{10 < \text{pore} < 100}$, and $V_{\text{pore} > 100}$ are the volume fractions of porosity for pores with mean pore radii, r_{pore} , less than 10 nm, between 10 and 100 nm, and greater than 100 nm, respectively.

The analytical model chosen for the mapping between porosity and compressive strength was based upon Kumar and Bhattacharjee [42], which developed a functional form of f_c based on Griffith model of fracture [43]. The function form starts with the tensile stress required for fracture of a brittle material, i.e.,

$$f_t = \sqrt{\frac{2ET}{\pi a}}, \quad (14)$$

where E is the effective modulus of elasticity for the porous material, T is the effective fracture surface energy for the porous material, and a is the half-crack length. Two assumptions were required to incorporate porosity. First, it was assumed that the effective modulus is $E = E_0(1 - V_{\text{pore}})$, where E_0 is the modulus of elasticity for the material without porosity.

Fig. 17 Comparison of dissipated energy density, G , as calculated by the model at the multiple fiber length scale and the fitting linear regression. The solid black line represents a one-to-one relation, and the dashed gray lines above and below the black line represent errors of $\pm 10\%$

Fig. 18 a Fitting of material constant K for the compressive strength as a function of the volume fraction of pores, V_{pore} , mean pore radius, r_{pore} , and mass ratio of water to cementitious materials, w/cm . **b** Comparison of f_c as calculated by Eq. (18) to f_c as experimentally measured. The solid black line represents a one-to-one relation, and the dashed gray lines represent errors of $\pm 10\%$ (Color figure online)

Second, it was assumed that $T = T_0(1 - V_{\text{pore}})$, where T_0 is the fracture surface energy for the material without porosity. The effects of hydration in Kumar and Bhattacharjee's model were incorporated by introducing the mass fraction of cementitious materials, M_c , such that Eq. (14) is expressed as

$$f_t = k_1 M_c \frac{(1 - V_{\text{pore}})}{\sqrt{r_{\text{pore}}}}, \quad (15)$$

where k_1 is a constant depending upon E_0 and T_0 . Finally, the unconfined compressive strength was assumed to be proportional to f_t , resulting in

$$f_c = k_2 M_c \frac{(1 - V_{\text{pore}})}{\sqrt{r_{\text{pore}}}}, \quad (16)$$

where k_2 is a different material constant. The model was used by Kumar and Bhattacharjee [42] to fit experimental data with $13.6 \leq f_c \leq 43.2$ MPa and $0.38 \leq w/cm \leq 0.65$. Here, the model is adapted for matrices with lower w/cm and greater compressive strengths by replacing M_c with $\frac{1}{w/cm}$, resulting in

$$f_c = K \frac{(1 - V_{\text{pore}})}{w/cm \sqrt{r_{\text{pore}}}}. \quad (17)$$

The material constant K was determined by fitting experimental data of Kumar and Bhattacharjee [42] and Klobes, Rübner, Hempel, and Prinz [25]. Figure 18a shows the fit of the linear regression determining $K = 99.3 \text{ MPa}\sqrt{\text{nm}}$, thus resulting in the nominal relation

$$f_c = 99.3 \frac{1 - V_{\text{pore}}}{w/cm \sqrt{r_{\text{pore}}}}. \quad (18)$$

Figure 18b compares measured f_c to the prediction of the model. The solid black line has a slope of one, the two gray lines have slopes $\pm 10\%$ from unity.

Mapping Between Porosity and Tensile Response

The tensile response of UHPCs may be measured via ASTM 1609 flexural tests [44], ASTM C496 split cylinder [45], or direct tension tests. Due to the difficulty and recent emergence of the direct tensile tests, there is a paucity of data in literature regarding direct tensile tests, porosity, and pore size distribution. Therefore, an intermediate relation between tensile strength and compressive strength will be used to determine a relation between tensile strength and porosity.

The mapping between tensile strength and compressive strength was assumed to be a power law relation, i.e., $f_t = c_0(f_c)^n$, where c_0 and n are material parameters to be determined from experiments, from which n is typically in the range between 0.5 and 0.75 for concretes with f_c between 7 and 69 MPa [46]. Here, the power law relation was calibrated to data from Garas-Yanni [47], Pul [48], and Zheng, Kwan, and Lee [49] as shown in Fig. 19. In Fig. 19, the black line represents the nominal relation between f_t and f_c , i.e.,

$$f_t = 0.177(f_c)^{0.74}. \quad (19)$$

Fig. 19 Relation between uniaxial tensile strength, f_t , and unconfined compressive strength, f_c (Color figure online)

Fig. 20 Model of blast loading at the structural length scale (Color figure online)

The gray lines below and above the nominal relation represent the lower and upper functions, i.e.,

$$\begin{aligned} f_{t, \text{ lower}} &= 0.144(f_c)^{0.74}, \text{ and} \\ f_{t, \text{ upper}} &= 0.216(f_c)^{0.74}. \end{aligned} \quad (20)$$

Using Eq. (18), the nominal relation between f_t and V_{pore} , r_{pore} , and w/cm is expressed as

$$f_t = 0.177 \left(99.3 \frac{1-V_{\text{pore}}}{w/cm \sqrt{r_{\text{pore}}}} \right)^{0.74}, \quad (21)$$

and the lower and upper bounds of f_t are expressed as

$$\begin{aligned} f_{t, \text{ lower}} &= 0.144 \left(99.3 \frac{1-V_{\text{pore}}}{w/cm \sqrt{r_{\text{pore}}}} \right)^{0.74}, \text{ and} \\ f_{t, \text{ upper}} &= 0.216 \left(99.3 \frac{1-V_{\text{pore}}}{w/cm \sqrt{r_{\text{pore}}}} \right)^{0.74}. \end{aligned} \quad (22)$$

Property-Performance Mappings

Mapping Between Panel Thickness, Fiber-Reinforced Tensile Properties, and Blast Loading

Property-performance mappings in this case relate hierarchical material structure and properties to the design of a blast panel with specified ranged sets of performance requirements. The mapping between panel thickness, quasi-static maximum tensile strength of fiber-reinforced UHPC, quasi-static dissipated energy density of fiber-reinforced UHPC (deductive inputs) and the ability to withstand a blast load without

completely fracturing (deductive output) was estimated via a 3D FE model at the structural length scale. As shown in Fig. 20, the model at the structural length scale consisted of a panel (shades of red), two back restraints (gray), and two front restraints (gray). The panel consisted of bulk and cohesive elements to account for compressive and tensile responses, respectively. The shown face of the panel (i.e., positive x_3 direction) is denoted as the proximal face; the back face of the panel (i.e., negative x_3 direction, not shown in Fig. 20) is denoted as the distal face. The positive and negative x_1 faces of the back and front restraints were fixed; the positive x_2 face of the upper back restraint was fixed; and the negative x_2 face of the lower restraint was fixed. In this manner, the boundary conditions are similar to, but not identical to, “simply supported” boundary conditions.

The model included a strain-rate sensitive constitutive relation for the fiber-reinforced UHPC [39] and was simulated within Abaqus/Explicit v6.10 [33]. Invariance of dissipated energy density and damage initiation stress at the crack plane guided the scale transition from the intermediate length scale to the structural length scale.

The UHPC panel’s performance, i.e., either survives or completely fractures after application of the impulse load, was estimated using a computational model at the structural length scale, which is shown here in Fig. 20. In the model, the blast load was applied to the proximal face with a maximum pressure $p_{\text{max}} = (2I)/(15 \text{ ms})$ at 0 ms and linearly decreased to 0 Pa at 15 ms, where I is the impulse. Further details and a comparison of empirical data and numerical simulations at the structural and multiple fiber length scales both employing 2% fiber volume fractions of 14-mm-long by 0.185-mm-diameter fibers and subjected to a 2.05-MPa-ms impulse resulted in similar critical impulses required to fracture a panel, associated displacements at the mid-height of the panel, fracture patterns, and evolution of fracture were shown in Ellis et al. [39]. Figure 21 compares the displacements and fracture evolution of a numerical simulation and experiment of a UHPC panel with 2% fiber volume fractions subject to a 2.05-MPa-ms impulse.

Response Surfaces

The model at the structural length scale was employed to estimate the critical specific impulse, defined here as the mean of the maximum impulse that the numerically simulated panel could survive and the minimum impulse that the numerically simulated panel could not survive, within a 36-data-point parametric space encompassing $G = [20: 20: 80]$ (kJ/m²), $T^o = [14.7, 20, 40]$ (MPa), and panel thickness $t_{\text{panel}} = [38.1: 12.7: 63.5]$ (mm). A bisection method with a minimum discretization of 0.25 MPa-ms was employed to determine the maximum impulse that the simulated panel could survive and the minimum impulse that would cause the simulated panel to completely fracture.

Fig. 21 Comparison of displacements and fracture patterns for a numerically simulated panel and an experimental UHPC panel, both subject to a single 2.05-ms impulse load. The simulated panel assumed

and the experimental panel employed 14-mm-long by 0.185-mm-diameter fibers loaded at 2% fiber volume fraction (Color figure online)

Fig. 22 Simulated critical specific impulses for panel thicknesses of **a** 38.1 mm, **b** 50.8 mm, and **c** 63.5 mm (Color figure online)

Fig. 23 Comparison of the critical specific impulse I_{cr} as calculated by the blast panel structural length scale (BPSLS) model and Eq. (23). The solid black line represents a one-to-one relation, and the dashed gray lines above and below the black line represent errors of $\pm 10\%$

Figures 22a–c show the calculated critical specific impulses for $t_{\text{panel}} = 38.1, 50.8, \text{ and } 63.5 \text{ mm}$, respectively. Figure 22 generally shows that the estimated critical specific impulse generally increases with dissipated energy density, quasi-static tensile strength, and panel thickness; however, the numerically estimated critical specific impulse for the $T^o = 14.7 \text{ MPa}$, $G = 80 \text{ kJ/m}^2$, and $t_{\text{panel}} = 63.5 \text{ mm}$ data point was higher than the general trend suggests. Results presented in Ellis [24] suggest that this higher than expected critical specific impulse resulted from a change in fracture behavior of the UHPC panel from brittle to ductile. Physical experiments have yet to be conducted that support or contradict the numerically observed brittle to ductile transition.

Excluding the critical specific impulse for $T^o = 14.7 \text{ MPa}$, $G = 80 \text{ kJ/m}^2$, $t_{\text{panel}} = 63.5 \text{ mm}$, a linear regression analysis of the data shown in Fig. 22 generates the following response function for critical specific impulse:

$$I_{cr} = -0.857 + 0.0262t_{\text{panel}} + 6.51 \times 10^{-4}t_{\text{panel}}T^o + 4.22 \times 10^{-4}t_{\text{panel}}G. \quad (23)$$

The correlation between Eq. (23) and data in Fig. 22 are shown in Fig. 23. The solid black line represents the regression shown in Eq. (23), and the dashed gray lines above and below the black line represent errors of $\pm 10\%$.

Results and Discussion

Feasible Design Space

The feasible properties, structures, and processes satisfying the minimum 1.5-MPa-ms blast loading performance requirement were determined via IDEM. Starting at the coarsest length scale containing a single performance requirement, the clarified design task is shown in Fig. 24. In Fig. 24, the design space is shown at the top of the figure and discretized according to the [minimum: step size: maximum] convention

specified previously. For example, the quasi-static tensile strength, T^o , has a lower bound of 10 MPa, an increment of 2 MPa, and a maximum value of 20 MPa. Therefore, the discretized quasi-static tensile strength space is 10, 12, 14, 16, 18, and 20 MPa. The critical specific impulse response is the regression previously defined in Eq. (23) with a $\pm 10\%$ uncertainty in the metamodel as shown in Fig. 23. A $\pm 10\%$ uncertainty was assumed for the discretization levels of the input variables within the design space.

With the design task clarified, the IDEM algorithm determined the feasible design space and boundary of the feasible design space as shown in Fig. 25. In Fig. 25, sets of discrete input values satisfying the performance requirements are shown as small teal spheres; sets of discrete input values at the boundary, i.e., $HDEMI_{I=1.5 \text{ MPa-ms}} = 1$, are shown as large black spheres. Infeasible points, i.e., $HDEMI_{I=1.5 \text{ MPa-ms}} < 1$, are not shown in Fig. 25.

Figure 26 clarifies the design task to determine feasible matrix tensile strength, fiber pitch, panel thickness, and fiber volume fractions. The feasible space of the two responses, quasi-static tensile strength of the fiber-reinforced microstructure, T^o , and dissipated energy density, G , appears in Fig. 25. A $\pm 10\%$ uncertainty was assumed for the discretization levels of the input variables within the design space.

The clarified design task from Fig. 26 facilitates IDEM to determine the feasible design space, as shown in Fig. 27. The empty scatter plot in Fig. 27a indicates that no feasible points were identified.

The remainder of this section provides the clarified design task for the material structures and processes in Figs. 28 and 30, respectively. The feasible spaces and boundaries of the feasible spaces for structures and processes are shown in Figs. 29 and 31, respectively. Note that for the clarification of the design task to define the feasible processing space shown in Fig. 30 and the feasible processing design space in Fig. 31, it is assumed that the UHPC has been thermally cured at 90°C ; no points were feasible with a curing temperature of 20°C .

Minimal Mass Within the Feasible Design Space

Determining the minimum mass of a panel within the feasible design space is important for several reasons. First, the mass of the UHPC panel may impact the transportation of UHPC panels either from the construction site to the final structure or if the final structure is intended to be mobile. Second, the mass of UHPC panels may influence the design and load-carrying capability of the structure supporting the panels, thus causing the overall costs of a structure incorporating the UHPC panels to increase. Therefore, it is important to understand material and structural designs that satisfy the performance requirements while minimizing mass of the panel.

Fig. 24 Clarification of design task for impulsive loading of UHPC panel

Design Space	Quasi-static tensile strength, T^o Dissipated energy density, G Panel thickness, t_{panel}	$x_1 = [10 : 2 : 20]$ (MPa) $x_2 = [20 : 5 : 100]$ (kJ/m ²) $x_3 = [39 : 6 : 61]$ (mm)
Response	$I_{cr}(T^o, G, t_{panel}) = -0.857 + 0.0262 t_{panel} + 6.51 \times 10^{-4} t_{panel} T^o + 4.22 \times 10^{-4} t_{panel} G$	
Uncertainty	$\Delta x_1 = \pm 10\% x_1$ $\Delta x_2 = \pm 10\% x_2$ $\Delta x_3 = \pm 10\% x_3$ $I_{cr, upper}(T^o, G, t) = 1.1 I_{cr}$ $I_{cr, lower}(T^o, G, t) = 0.9 I_{cr}$	
Fixed Parameters	Applied impulse ($I = 1.5$ MPa-ms)	
Goal	The UHPC panel should survive (i.e., not completely fracture) one loading at the specified applied impulse.	
Task Objectives	Identify the feasible space of T^o – G – t_{panel} (i.e., $HDEMI_{I=1.5 \text{ MPa-ms}} \geq 1$) such that the requirement is satisfied. The feasible T^o – G – t_{panel} space will define the output constraint at the multiple fiber length scale.	

A rule of mixtures approach is utilized to calculate the mass density of the UHPC material, i.e.,

$$\rho_{UHPC} = V_{\text{fiber}} \rho_{\text{fiber}} + (1 - V_{\text{fiber}}) \left(V_{\text{cem}} \rho_{\text{cem}} + V_{\text{SF}} \rho_{\text{SF}} + V_{\text{agg}} \rho_{\text{agg}} + \frac{w/cm}{\rho_{\text{water}}} (V_{\text{cem}} \rho_{\text{cem}} + V_{\text{SF}} \rho_{\text{SF}}) \right), \quad (24)$$

where V_i are the volume fractions of the i th materials, and ρ_i are the mass densities of the i th materials. In Eq. (24), the volume fractions and water to cement ratio are determined from the feasible design space, and the mass densities are listed in Table 2. The mass of the panel is

$$\text{mass} = \rho_{UHPC} t_{\text{panel}} w_{\text{panel}} h_{\text{panel}}, \quad (25)$$

where t_{panel} is the thickness of the panel which can vary between 39 and 63 mm, and w_{panel} and h_{panel} are the width and height of the panel fixed to 1625.6 and 863.6 mm, respectively.

The mass of the panel was calculated using Eqs. (24) and (25) for each previously identified feasible and boundary point. The minimum mass of all feasible and boundary points was then found via the constrained optimization problem:

Fig. 25 Feasible UHPC properties and panel thicknesses which survive a 1.5-MPa-ms specific impulse blast load. Boundary points are shown for clarity (Color figure online)

Fig. 26 Clarification of design task to determine matrix tensile strength, fiber pitch, panel thickness, and fiber volume fraction to satisfy required quasi-static tensile strength and dissipated energy density

Design Space	Matrix tensile strength, f_t Axial length per revolution, $pitch$ Panel thickness, t_{panel} Fiber volume fraction, V_{fiber}	$x_1 = [5 : 0.5 : 9]$ (MPa) $x_2 = [6 : 3 : 36]$ (mm) $x_3 = [39 : 6 : 63]$ (mm) $x_4 = [1.25 : 0.25 : 2]$ (%)
Responses	$T^o(f_t, pitch, V_{fiber}) = 3.47 + 0.569(1 - V_{fiber})f_t + 4830 <V_{fiber} - 0.00866> pitch^{-0.937}$ $G(f_t, pitch, V_{fiber}) = 0.166 + 4320 V_{fiber} - 62.4 V_{fiber} pitch$	
Uncertainty	$\Delta x_1 = [\pm 10\%]$ $\Delta x_2 = [\pm 10\%]$ $\Delta x_3 = [\pm 10\%]$ $\Delta x_4 = [\pm 10\%]$ $T^o_{upper}(f_t, pitch, V_{fiber}) = 1.25 T^o$ $T^o_{lower}(f_t, pitch, V_{fiber}) = 0.75 T^o$ $G_{upper}(f_t, pitch, V_{fiber}) = 1.1 G$ $G_{lower}(f_t, pitch, V_{fiber}) = 0.9 G$	
Fixed Parameters	Fiber length Effective fiber diameter	$L_{fiber} = 25$ mm $d_f = 0.5$ mm
Goal	The combination f_t – $pitch$ – t_{panel} – V_{fiber} should satisfy the requirements quasi-static tensile strength, T^o , and dissipated energy density, G , of the fiber-reinforced composite.	
Task Objectives	Identify the f_t – $pitch$ – t_{panel} – V_{fiber} input space such that $HDEMI_{T^o} \geq 1$ and $HDEMI_G \geq 1$.	

Fig. 27 Feasible f_t – $pitch$ – t_{panel} – V_{fiber} input space that satisfies the identified T^o – G – t_{panel} feasible space identified in Fig. 25 (Color figure online)

Fig. 28 Clarification of design task to determine material structural attributes satisfying the non-fiber-reinforced tensile strength of the matrix

Design Space	Water to cementitious material ratio, w/cm	$x_1 = [0.15 : 0.05 : 0.45]$ ()
	Volume fraction of pores, V_{pore}	$x_2 = [0.01 : 0.05 : 0.51]$ ()
	Mean pore radii, r_{pore}	$x_3 = [1 : 5 : 31]$ (nm)
Responses	$f_t(w/cm, V_{pore}, r_{pore}) = 0.177 \left(99.3 \frac{1 - V_{pore}}{w/cm \sqrt{r_{pore}}} \right)^{0.74}$	
Uncertainty	$\Delta x_1 = [\pm 5\%]$ $\Delta x_2 = [\pm 5\%]$ $\Delta x_3 = [\pm 10\%]$	
	$f_{t,upper}(w/cm, V_{pore}, r_{pore}) = 0.216 \left(99.3 \frac{1 - V_{pore}}{w/cm \sqrt{r_{pore}}} \right)^{0.74}$	
	$f_{t,lower}(w/cm, V_{pore}, r_{pore}) = 0.144 \left(99.3 \frac{1 - V_{pore}}{w/cm \sqrt{r_{pore}}} \right)^{0.74}$	
Goal	The combination $w/cm - V_{pore} - r_{pore}$ should satisfy the requirements for non-fiber-reinforced matrix tensile strength, f_t .	
Task Objectives	Identify the $w/cm - V_{pore} - r_{pore}$ input space such that $HDEMI_{f_t} \geq 1$.	

Minimize : mass
 Subject to : $HDEMI_i \geq 1$
 $39 \leq t_{panel} \text{ (mm)} \leq 63$
 $6 \leq \text{pitch (mm)} \leq 36$
 $1.25 \leq V_{fiber} \leq 2\%$
 $0.22 \leq w/cm \leq 0.30$
 $0.10 \leq V_{cem} \leq 0.20$
 $0.01 \leq V_{SF} \leq 0.05$
 $T_{cure} = 20, 90^\circ\text{C}$

(26)

Results of the constrained optimization problem using data determined from a robust design approach indicate that a 157 kg UHPC panel can survive a 1.5 MPa-ms specific impulse. The preferred material design contains $V_{cem} = 0.196$, $V_{SF} = 0.049$, $w/cm = 0.29$, and $V_{agg} = 0.522$, and $V_{fiber} = 0.020$ of triangular cross-sectional fibers that have been twisted to a 6-mm pitch. After curing at 90°C , the matrix has a 7-MPa uniaxial tensile strength. Using the mass densities listed in Table 2, the UHPC material design uses 618 kg of Portland

Fig. 29 Feasible $w/cm - V_{pore} - r_{pore}$ input space that satisfies the specified uniaxial tensile strength of the matrix, f_t , for $5 \leq f_t \leq 8$ MPa (Color figure online)

Fig. 30 Clarification of design task to determine material processes satisfying the structure performance requirements

Design Space	Curing temperature, T_{cure} Volume fraction cement, V_{cem} Volume fraction silica fume, V_{SF} Water to cementitious material ratio, w/cm	$x_1 = [20, 90] (^{\circ}\text{C})$ $x_2 = [0.10 : 0.02 : 0.20] ()$ $x_3 = [0.01 : 0.01 : 0.05] ()$ $x_4 = [0.20 : 0.02 : 0.30] ()$
Responses	$V_{pore}(w/cm, V_{cem}, V_{SF}) = -0.00398 - 0.000167T_{cure} + 0.201V_{cem} + 0.193V_{SF} + 0.298w/cm$ $- 0.000761T_{cure}V_{cem} - 0.000735T_{cure}V_{SF} - 0.00198T_{cure}w/cm$ $- 0.315V_{cem}^2 - 0.558V_{cem}V_{SF} + 1.37V_{cem}w/cm + 1.08V_{SF}w/cm$ $- 0.165w/cm^2$ $r_{pore}(w/cm, V_{cem}, V_{SF}) = 70.9 - 0.76T_{cure} - 71.5V_{cem} - 91.1V_{SF} - 16.8w/cm$ $+ 1.10T_{cure}V_{cem} + 1.33T_{cure}V_{SF} + 0.307T_{cure}w/cm - 31.9V_{cem}^2$ $- 309V_{cem}V_{SF} - 65.2V_{cem}w/cm - 64.5V_{SF}^2 - 78.3V_{SF}w/cm$	
Uncertainty	$\Delta x_1 = [\pm 0\%]$ $\Delta x_2 = [\pm 5\%]$ $\Delta x_3 = [\pm 5\%]$ $\Delta x_4 = [\pm 5\%]$ $V_{pore, upper}(w/cm, V_{cem}, V_{SF}) = 1.1 V_{pore}$ $V_{pore, lower}(w/cm, V_{cem}, V_{SF}) = 0.9 V_{pore}$ $r_{pore, upper}(w/cm, V_{cem}, V_{SF}) = 1.15 r_{pore}$ $r_{pore, lower}(w/cm, V_{cem}, V_{SF}) = 0.85 r_{pore}$	
Fixed Parameters	gradation of aggregate $\rho_{cem} = 3,150 \text{ kg/m}^3$, $\rho_{SF} = 2,200 \text{ kg/m}^3$ $T_{cure} = 90 ^{\circ}\text{C}$	
Goal	The combination $T_{cure}-V_{cem}-V_{SF}-w/cm$ should satisfy the requirements for volume fraction of porosity, V_{pore} , and average pore radius, r_{pore}	
Task Objectives	Identify the $T_{cure}-V_{cem}-V_{SF}-w/cm$ input space such that $HDEMI_{V_{pore}} \geq 1$, and $HDEMI_{r_{pore}} \geq 1$.	

Fig. 31 Feasible $V_{cem} - V_{SF} - w/cm$ input space that satisfies the specified uniaxial tensile strength of the matrix, f_t , for $5 \leq f_t \leq 8$ MPa and $T_{cure} = 90 ^{\circ}\text{C}$ (Color figure online)

Table 2 Mass densities of UHPC constituents

ρ_{fiber} (kg/m ³)	ρ_{cem} (kg/m ³)	ρ_{SF} (kg/m ³)	ρ_{agg} (kg/m ³)	ρ_{water} (kg/m ³)
7850	3150	2200	2700	1000

cement, 108 kg of silica fume, 211 kg of water, and 1410 kg of aggregate. The feasible UHPC panel is 44.7 mm thick.

$$P_{\text{UHPC}} = V_{\text{fiber}}\rho_{\text{fiber}}P_{\text{fiber}} + (1 - V_{\text{fiber}}) \left(V_{\text{cem}}\rho_{\text{cem}}P_{\text{cem}} + V_{\text{SF}}\rho_{\text{SF}}P_{\text{SF}} + V_{\text{agg}}\rho_{\text{agg}}P_{\text{agg}} + w/cm(V_{\text{cem}}\rho_{\text{cem}} + V_{\text{SF}}\rho_{\text{SF}})P_{\text{water}} \right) \quad (28)$$

defines the costs of the UHPC per unit volume. In Eq. (28), P_i is the cost of the i th material per kilogram, with individual values of P_i are listed in US dollars (USD) per kilogram of material in Table 3. The cost density of fiber, P_{fiber} , was calculated assuming a 0.800 USD/kg cost density for raw steel, and that raw steel accounts for 40% of the costs of the manufactured fibers. The cost densities for Portland Cement, P_{cem} , silica fume, P_{SF} , and aggregate, P_{agg} , were sourced from the National Institute of Standards and Technology (NIST) Concrete Optimization Software Tool (COST) program [50]. The cost density of water, P_{water} , was assumed.

The minimum cost of the UHPC panel is determined through the constrained optimization problem

$$\begin{aligned} \text{Minimize :} & \quad \text{cost} \\ \text{Subject to :} & \quad \text{HDEMI}_i \geq 1 \\ & \quad 39 \leq t_{\text{panel}} \text{ (mm)} \leq 63 \\ & \quad 6 \leq \text{pitch (mm)} \leq 36 \\ & \quad 1.25 \leq V_{\text{fiber}} \leq 2\% \\ & \quad 0.22 \leq w/cm \leq 0.30 \\ & \quad 0.10 \leq V_{\text{cem}} \leq 0.20 \\ & \quad 0.01 \leq V_{\text{SF}} \leq 0.05 \\ & \quad T_{\text{cure}} = 20, 90^\circ \text{C} \end{aligned} \quad (29)$$

Results of the constrained optimization problem using feasible and boundary data points from IDEM indicate that preferred minimized cost UHPC panel costs \$23.58 per panel, or \$347/m³. The preferred material design contains $V_{\text{cem}} = 0.10$, $V_{\text{SF}} = 0.01$, $w/cm = 0.23$, and $V_{\text{agg}} = 0.797$, and $V_{\text{fiber}} = 0.0175$ of fibers having triangular cross sections that have been twisted to a 6-mm

Minimal Cost Within the Feasible Design Space

In addition to determining minimal mass of all possible feasible designs, other objective functions can be used. For example, a cost objective function

$$\text{Cost} = P_{\text{UHPC}} t_{\text{panel}} w_{\text{panel}} h_{\text{panel}} \quad (27)$$

can be defined, where the cost density of UHPC

pitch. The matrix has a 7-MPa uniaxial tensile strength, created by curing a mixture of at 90 °C. Using the mass densities listed in Table 2, the UHPC material design uses 315 kg of Portland cement, 22 kg of silica fume, 78 kg of water, and 2150 kg of aggregate representing a 2-mm maximum aggregate size sand mixed with quartz powder. The feasible UHPC panel is 48.4 mm thick.

Conclusions

A systematic *material design exploration process* was employed to design a hierarchically structured ultra-high-performance concrete (UHPC) panel subject to blast loading. This design exploration process consisted of bottom-up deductive mappings constructed from validated hierarchical multiscale models and analytical expressions, along with projected uncertainty, and top-down inductive decision pathways facilitated by the inverse design exploration method (IDEM). The assumed set of process-structure-property-performance (PSPP) mappings considered micro-, meso-, and macro-scale mappings across four spaces, seven design variables (panel thickness, fiber pitch, water to cementitious material ratio, curing temperature, and volume fractions of fibers, cement, and silica fume), and eight intermediate variables (pore volume fraction, mean pore radius, fiber end slip, fiber pullout force, quasi-static tensile strength of non-fiber-reinforced cementitious matrix, quasi-static compressive strength of non-fiber-reinforced cementitious matrix, quasi-static tensile strength of fiber-reinforced UHPC, and dissipated energy density of fiber-reinforced UHPC).

Table 3 Cost densities of UHPC constituents

P_{fiber} (USD/kg)	P_{cem} (USD/kg)	P_{SF} (USD/kg)	P_{agg} (USD/kg)	P_{water} (USD/kg)
2.00	0.081	0.88	0.013	0.0004

Implementation of the materials design process for the blast panel application proceeded by the following steps:

- (i) Defining a set of PSPP mappings
- (ii) Determining which analytical and experimental relations from literature could be employed as PSPP mappings
- (iii) Developing computational models to complete the set of PSPP mappings
- (iv) Validating the analytical, empirical, and numerical models
- (v) Generating metamodels or response surfaces and estimating error or uncertainty associated with each response function
- (vi) Determining ranged sets of design variable values within the feasible domain via IDEM, defining mass and cost objective functions, and determining preferred material designs

The choice of mass and cost objective functions and the resulting preferred material designs highlight the challenges associated with materials design. The feasible domain (i.e., ranged sets of values of design variables such that the UHPC panel withstands a 1.5-MPa-ms blast load) were determined via IDEM, which consists of three steps: discretize input variables, project discretized sets of input variables with account of uncertainty to a range in the output space, and determine which sets of discrete input values satisfy the output space requirement(s). When recursively applied, these three steps allow for robust searching of hierarchical design problems. The advantages of this approach are the identification of ranged sets of design variables values and the ability to account for propagated uncertainty. Although the IDEM algorithm was suitable for this case, it can be extended to admit concave feasible domains, multiple feasible domains within a parametric space, or feasible domains that are not simply connected.

The systematic application of IDEM presented here is significant for three reasons. First, this work demonstrates the utility and role of bottom-up, hierarchical multiscale modeling for UHPC materials and structures subject to blast loading. Second, this work demonstrates the concurrent design [2] of UHPC materials and structures subject to blast loading. Third, this work demonstrates a *materials design process* that can be employed for the simultaneous design of other materials for application-specific requirements. It is envisioned that through this *materials design process* or similar processes, the commercialization time for new material insertion into products can be reduced substantially.

5. List of Abbreviations and Symbols

α	degree of hydration
Δ	end slip
Δ_{offset}	offset end slip
d_f	effective fiber diameter
$d_{\min}$	minimum diameter particle
$d_{\max}$	maximum diameter particle
f_c	quasi-static compressive strength of non-fiber-reinforced cementitious matrix
f_t	quasi-static tensile strength of non-fiber reinforced cementitious matrix
E	modulus of elasticity
E_0	modulus of elasticity without porosity
$G_{n,s,t}$	dissipated energy density of fiber-reinforced UHPC in n , s , and t directions
I	applied impulse
λ	fiber aspect ratio equal L_f/d_f
L_e	fiber embedded length
$L_{e,\max}$	maximum fiber embedded length
L_f	fiber length
L_{free}	fiber free length
m_{agg}	mass of aggregate per cubic meter of concrete
M_c	mass fraction of cementitious materials
π	ratio of the circumference to the diameter of a circle
$p_{\max}$	maximum applied pressure
P	pullout force of a single fiber
$P_{\text{cap/paste}}$	volume fraction of capillary pores to cement paste
$P_{\text{gel/paste}}$	volume fraction of gel pores to cement paste
$P_{\max}$	maximum porosity in the ITZ
P_{ITZ}	ratio of porosity volume in ITZ to volume of the ITZ
ρ_{agg}	density of aggregate
ρ_{cem}	density of cement
ρ_{SF}	density of silica fume
ρ_{water}	density of water
$r_{\text{cap, paste}}$	characteristic radii of capillary porosity within the bulk paste
$r_{\text{cap, ITZ}}$	characteristic radii of capillary porosity within the ITZ
$r_{\text{gel, paste}}$	characteristic radii of gel porosity within the bulk paste
$r_{\text{gel, ITZ}}$	characteristic radii of gel porosity within the ITZ
r_{pore}	mean pore radii of hardened cement paste
sg_{cem}	specific gravity of cement
T_{cure}	curing temperature
T^o	quasi-static tensile strength of fiber-reinforced UHPC
t_{ITZ}	thickness of ITZ
t_{panel}	panel thickness
V_{agg}	aggregate volume fraction
V_c	volume of capillary pores

$V_{\text{cap, ITZ}}$	volume fraction of capillary porosity within the ITZ
$V_{\text{cap, paste}}$	volume fraction of capillary porosity within the bulk paste
V_{cem}	Portland cement volume fraction
V_{fiber}	fiber volume fraction
V_g	volume of gel pores
$V_{\text{gel, paste}}$	volume fraction of gel porosity within the bulk paste
$V_{\text{gel, ITZ}}$	volume fraction of gel porosity within the ITZ
V_{hp}	volume of hydration products
V_{ITZ}	ITZ volume fraction
V_p	initial volume of cement paste
V_{paste}	bulk paste volume fraction
V_{pore}	pore volume fraction
V_{SF}	silica fume volume fraction
$V_{\text{SF, max}}$	maximum possible volume fraction of silica fume
V_u	volume of un-hydrated cement
x_i	i^{th} design variable
Δx_i	uncertainty in i^{th} design variable
w_g	mass of water in the gel pores
w_{min}	minimum ratio of mass of water to the mass of original cement
w_n	mass of non-evaporable water
w/c	water to cement ratio by weight
w/cm	water to cementitious material ratio by weight
BPSLS	blast panel structural length scale
CSH	calcium-silicate-hydrate
FA	fly ash
FE	finite element
HDEMI	hyper-dimensional error margin index
HSC	high-strength concrete
HWRA	high-range water reducing agent
IDEM	inductive design exploration method
ITZ	interfacial transition zone
LPM	linear packing model
MCTP	mix constituents and curing temperature to porosity
MIP	mercury infusion porosimetry
Mmt	10^6 metric tons
N	total number of aggregates in a unit volume
NSC	normal-strength concrete
PC	Portland cement
<i>pitch</i>	fiber pitch
PSPP	process-structure-property-performance
RBSM	rigid body-spring model
SF	silica fume
UHPC	ultra-high-performance concrete

Acknowledgments The authors acknowledge Dr. Beverly P. DiPaolo and the Engineer Research and Development Center, US Army Corps of Engineers for experimental data used to validate the multiscale models.

Dr. Min Zhou of the Georgia Institute of Technology is acknowledged for suggestions regarding the multiscale modeling of cementitious materials.

This work was sponsored by the Department of Homeland Security, Science and Technology Directorate, Infrastructure Protection and Disaster Management Division: Ms. Mila Kennett, Program Manager. The research was performed under the direction of Dr. Beverly P. DiPaolo, Engineer Research and Development Center, US Army Corps of Engineers. Permission to publish was granted by the Director, Geotechnical and Structures Laboratory, ERDC. Approved for public release; distribution is unlimited.

Authors' Contributions BDE conducted the multiscale modeling and inductive design exploration method (IDEM) computational analyses, coded IDEM in MATLAB, and drafted and edited the manuscript. DLM conceived the study, supervised the study's design, and contributed to the final manuscript. BDE and DLM read and approved the final manuscript.

Compliance with Ethical Standards

Competing Interests The authors declare that they have no competing interests.

Funding Funding for the design of the study; collection, analysis, and interpretation of the data; and writing the manuscript was provided by the Engineer Research and Development Center, US Army Corps of Engineers.

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