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MODERN CHALLENGES AND PROSPECTS IN MODELING COMPLEX HEAT AND MASS TRANSFER PROCESSES

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Abstract

Reliable modeling of coup led heat and mas s transfer is a cornerstone of technolog ical pr ogress in energy systems, advanced manufac turing, e nvironmental engineering, and biomedical applications. However, as modern systems increasingly exhibit mul tiscale behavio r, material heteroge n eit y, and strong interphysics interactions, the limitations of traditional modeling strategies a re becoming increasingly apparent . This paper presents a detailed analysis of the key ch allenges facing t his field, along with a structured assessment o f new computational and methodological approac h e s devel oped to address them. The analysis f ocuses on several cri tical obstacles, including the exponential growth in c omplexit y in multiscale formulations, accurate representation of phase transit ion boundaries, mo deling and ch aracterization of advanced and unconventional mate ri als, and persiste nt shortcomings in high-quali ty valid ation data. Based on a synthes is of rec ent advan c es in hig h-performance co mputing, physics-based machine learning, and hybri d model ing metho ds, this paper identifies promisi ng avenues for overcoming these limitati ons. Resul ts from represe ntative case studies demonstrate that surrogate a nd reduced-order models can provide an order of magnit u de increase in computational efficiency, while comparative evaluations hi ghlight the rapidly expanding role of data-drive n met hods in predictive modeling. We argue that future progress in heat and mass tra nsfer modeling wil l depend on th e development of integrated systems that tightl y couple fundamentally based models with dat a-driven components, in corporate rigorous unce rtainty quantifi cation, and enable th e creation of experimentally validated digital twins . This integration signals a fund amental shif t from p ur ely physical simulations to ad ap tive, intelligent computing systems cap ab le o f continuous improvement.

Key challenges shaping contemporary modeling

Contemporar y heat and mass tra nsfer modeling is const rained by a set of tig htly coupled challenges that defi ne the limi ts of cu rre nt computationa l capabilitie s. A primary d ifficulty arises from the extreme multi-scale character of the g overning phenomena. Relevant processes span from nanoscale interfacial effects to full system beh avior, creating a fundamental modeling barr ier. For insta n ce, accur ately simulating metal ad d itive manufacturing demands spatial coverage acro ss roughly five

order s of ma gnitude—f rom micron- scale laser–material interactions to centimeter-scale components—and tem poral res olution extend ing over as many as seve nteen orders, from nanosecond laser pulses to the long- term evolution of residual stresses over years. This vast scale disparity leads to rapidly escalati ng computational costs: direct numeric al simulations of porous structur es with approximately 10^6 cel ls can require on the order of 10^4 CPU hours, whereas homogenized m odels re duce the cost to ab out 1 0^2 hours but at the expense of 15– 40% loss in accuracy for interfacial transport predictions. Additional complexity is introduced by phase-change pro cesse s and moving boundaries, w hich inv olve strong nonlinearities that undermine traditional empirical c orrelations. In boiling heat transfer, for exa mple, standar d predictive mode ls can yield errors exceeding 50% w hen applied to micro-str uctured surfa ces, posin g serious safety concerns. Interface - capturi ng techniques such as the Volume-of -Flui d m ethod typically suffer from cumulative mass co nservat i on errors of 1–5% per time step. A t the same time, critical microscale effects near co nt act lines often re quire mo lecular dyna mi cs simulation s, which are r estricted to domains on the or der of 100 n m, l eavi ng a persist ent and unresolved gap between atomis tic and continuum descriptions. In multip hase appl ica tions such as spr ay cooling, the problem is further amplified by high sensitivity to initial c onditions, where mod est uncertainties (e.g., ±10% in droplet diameter) can lead to variations of up to ±35% i n predicted heat flu x. Mate rial beha vi or adds y et another layer of difficulty . Many advanced m at erials deviate markedly fro m classical Fourier and Fick tran sport law s. Carbon nanot ube–based composites, fo r instance, can exhi bit thermal conductivity anisotrop y a pproaching 300%, while engineered metama terials may achieve effective thermal co nductivities reduced by as much as 70% co m pared to thei r base constitu ents. Biologica l tissue s present even greater variability, with porosity ranging from 20% to 90% and permeability spanning eight o rders of magnitude (10^{-1} ^{8} to 10^{-10} m^2). Su ch diversity necessitates material-specific constitutive formulations, as generalized correlations tend to fail severely beyond their calibration domains. These technica l ob sta cles are co mp ounded by a pervasive lack of reliable data. Although numerical simulat ions routinely generate massive datasets, rigorous experimental vali dation remains l imited. Analy ses of stud ies pu blished between 2018 an d 2 023 indicate that only about 32% include quantit a tive c omparisons wi th experiments, and just 18 % re port uncerta inty estimates for both numerical and experimental results. Experi mental techniques themselves impose additional constr aints: methods such as micro- PIV a nd infrared thermography are typically limited to spatial resolutions of around 10 µm an d tempor al resolu t i ons of approximately 1 ms, whic h are often coarser than tho se a chieva ble in simulations. Moreover, comprehensive material characterization across a range of operating conditions may require betwe en 10^3 a nd 10^4 individual measureme nts, re sulting in substantial time and co st barr iers th at hinder thorough model validation .

Table 1.

Quantitative Overview of Modern Modeling Challenges.

Challenge Category	Typical Scale Range	Computational Cost	Accuracy Limitation	Key Bottleneck
Multi-scale problems	10^{-6} to 10^0 m spatial, 10^{-9} to 10^8 s temporal	10^2–10^4 CPU hours	15–40% interface error	Scale coupling, computational expense

Phase-change dynamics	Interface thickness: 10^{-9}–10^{-6} m	10^{3}–10^{5} CPU hours	1–5% mass error/step	Moving boundaries, microphysics
Advanced materials	Property anisotropy: 100–300% variation	10^{1}–10^{3} CPU hours	20–50% correlation error	Non-classical behavior, heterogeneity
Data validation	Resolution gap: 10^{-1}–10^{2} μm, 10^{-6}–10^{-3} s	Experimental: 10^{2}–10^{4} points	10–25% measurement uncertainty	Access, cost, instrumentation limits

These interconnected problems—computational, physical, material, and empirical—create a self-perpetuating cycle in which model limitations limit understanding of the system, which in turn limits model improvement. Breaking this cycle requires not just incremental advances in individual areas, but also comprehensive approaches that simultaneously address multiple problematic aspects.

Modeling prospects for the drying process of black currant fruits

The modeling challenges described above have catalyzed dramatic changes in computational methods, the integration of data science, and algorithmic innovation, collectively offering ways to overcome traditional limitations. High-performance computing has dramatically expanded the boundaries of possible modeling, and exascale systems like the 1.7 exaFlops Frontier supercomputer have reduced the runtime of detailed turbulent combustion simulations from months to days. Heterogeneous architectures combining CPUs with GPUs and specialized accelerators have demonstrated particularly significant benefits, delivering 20-50x speedups for lattice Boltzmann simulations through massive parallelization of streaming collision processing operations. This hardware revolution enables previously intractable multiscale simulations, but computational power alone is not sufficient to address all challenges—algorithmic innovations must complement hardware advances. Regarding the fruit drying process, this study presents a mathematical model of blackcurrant drying in a microwave-assisted vacuum drying system. The model describes the interrelated heat and mass transfer mechanisms occurring during microwave vacuum drying and takes into account the influence of applied microwave energy and reduced pressure on moisture removal and temperature distribution within the material. The developed model, characterized by a high degree of detail, describes the blackcurrant fruit drying process and, therefore, includes a large number of adjustable parameters. Among these, three key process parameters were selected as having the greatest impact on drying efficiency and product quality: microwave power P, fruit layer thickness h, and atmospheric pressure p. Among the model output variables, the most important are three time-dependent functions:

- the average moisture content of the layer Wavg(t)
- the rate of change of the average moisture content dWavg(t)/dt
- the average temperature of the layer Tavg (t). The calculation of these functions is carried out using the following formulas:

$$W_{cp}(t) = \frac{\sum_{i=1}^{N_э} W_i^{t/\Delta t}}{N_э}, \quad (1)$$

$$\frac{dW_{cp}(t)}{dt} = \frac{\sum_{i=1}^{N_э} W_i^{t/\Delta t} - \sum_{i=1}^{N_э} W_i^{t/\Delta t - 1}}{N_э \Delta t}, \quad (2)$$

$$T_{cp}(t) = \frac{\sum_{i=1}^{N_э} T_i^{t/\Delta t}}{N_э}. \quad (3)$$

The relationship between the input parameters of the model and its output characteristics is schematically illustrated in Figure 2.

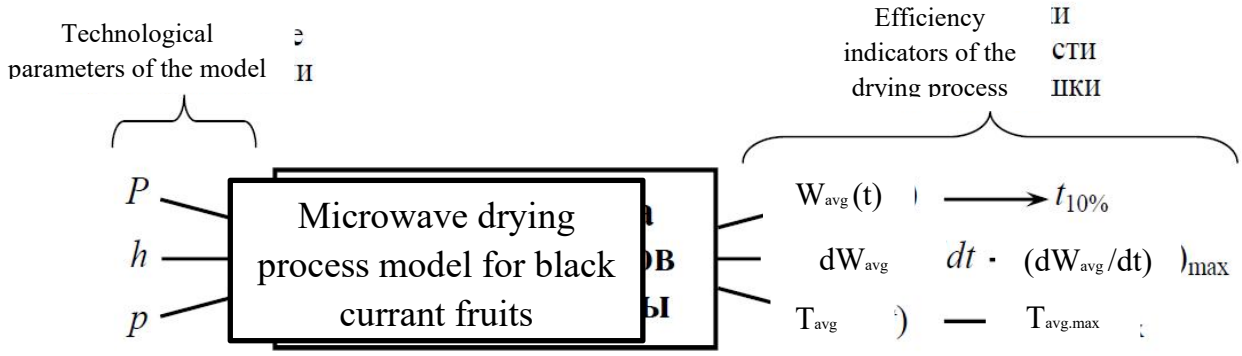

Figure 2. Formulation of the theoretical research problem.

Based on the proposed scheme (Figure 1), the theoretical study requires solving the following optimization problem [1–3]:

$$\begin{cases} t_{10\%}(P,h,p) \to \min; \\ \left(dW_{cp}/dt\right)_{\max}(P,h,p) \to \max; \\ T_{cp.\max}(P,h,p) \to \min. \end{cases}$$

Boundary conditions for the heat and mass transfer problems are defined by the following equations: (5, 6)

$$W_i^{\tau+1} = W_i^{\tau} - k_W \left(W_i^{\tau} - W_{\text{env}}^{\tau} \frac{p_{\text{atm}}}{p} \right) \Delta t, \quad (5)$$

$$T_i^{\tau+1} = T_i^{\tau} - \chi_T \left(T_i^{\tau} - T_{\text{env}}^{\tau} \right) \Delta t. \quad (6)$$

Key takeaways and future prospects: bridging challenges and solutions

The discussion presented in this a rti cle leads us to a key con clusi on: heat and mass transfer modeli ng is undergoing a transformational shift drive n by the need to address mode rn chal lenges such as multi scale phenomena, co mplex int erphase dynamics,

m a terial heterogeneity, and limited expe rimental d ata. Progress in this field is increasing ly driven not by in cremental refine ments of traditional continuum a pproac hes, but by the targeted integrati on of co mputation al physics, data-driven methodolog ies, an d rigorous uncertainty quantification wit hin holistic, i ntelligent systems. Remarkably, recent adv ances—illustrated by 50- to 1000-fold increases in compu tational efficienc y without sacrificing accuracy thanks to hybrid approaches combining phys ics and artificial int elligenc e—demo nstrate that these promises are not merely conc ept u al but lead to concrete, substantial impro vement s. This synthesis suggests that f uture practition ers will work less as specialist s in a single numerical method and more as systems architects coordinating mechanistic mo dels, surrogate data-based tools , and verifi c ation st rategies to solve problems previously consid ered intractable.

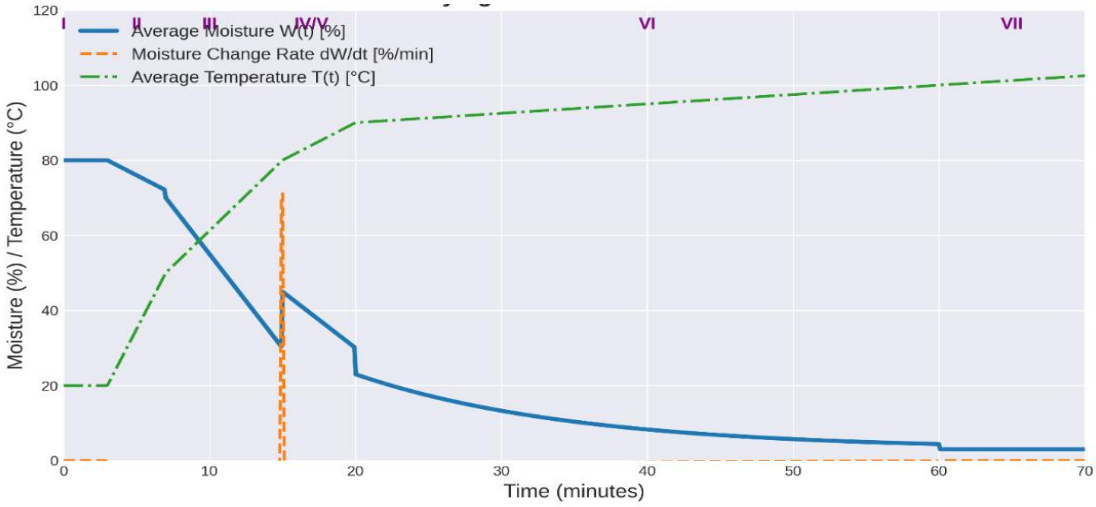

Figure. Microwave drying kinetics of black currant fruits.

The graph illustrates the microwave drying kinetics of black currant fruits over 70 minutes. It shows three key variables:

1. Average moisture content (W(t), blue solid line): starts at 80% and decreases rapidly during stage III (7–15 min), then gradually approaches a minimum of ~3–5% by stage VI.
2. Rate of moisture change (dW/dt, orange dashed line): peaks around 10 minutes, indicating the fastest dehydration, then declines to near zero as drying completes.
3. Average temperature (T(t), green dash-dot line): rises quickly from 20°C to ~90°C during the initial stages, then slowly increases to ~100–110°C in stage VII.

The stages I–VII are annotated above the graph, highlighting: initial state, rapid heating, rapid dehydration, slow dehydration, product layer consolidation, final drying, and post-drying heating.

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