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Validation of Pronghorn friction-dominated porous media thermal-hydraulics model with the SANA experiments

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ABSTRACT

A significant challenge in the core modeling of pebble bed reactors (PBRs) is the complex fuel-coolant structure. At the expense of approximating local flow and heat transfer effects, porous media models can provide medium-fidelity predictions of complicated thermal-fluid systems with significantly less computational cost than high-fidelity Computational Fluid Dynamics (CFD) models. This paper presents a new porous media code, Pronghorn – a fast-running core simulator intended to accelerate the design and analysis cycle for PBRs and provide boundary conditions for systems-level analysis. This paper describes the physical models in Pronghorn and demonstrates the capability of a friction-dominated model for predicting gas-cooled PBR decay heat removal by presenting simulation results for all 52 of the steady-state axisymmetric German SANA experiments, which include two different fluids and three different types of pebbles. The pebble temperature in all 52 cases is predicted with a mean error (predicted minus experimental) of +22.6 °C with standard deviation of 54.6 °C. To demonstrate Pronghorn's capability for modeling bed-to-plenum heat and mass transfer, one open-plenum SANA experimental case is also simulated. A code-to-code comparison with Flownex and GAMMA shows that Pronghorn is comparable in accuracy to other porous media simulation tools, with the additional advantages of 1) an arbitrary equation of state; 2) 3-D unstructured mesh capabilities; and 3) multiphysics coupling to other Multiphysics Object-Oriented Simulation Environment (MOOSE) applications. Finally, the effect of several porous media closure selections, in particular the porosity, the near-wall treatment for effective solid thermal conductivity, the interphase drag and heat transfer, and the fluid thermal dispersion, on temperature predictions are quantified.

1. Introduction

Pebble Bed Reactor (PBRs) are expected to display excellent heat removal characteristics due to graphite's capability for storing and transferring heat, the high failure temperatures of particle fuel, and the low power densities involved. However, a major challenge associated with the modeling of PBRs is the complex fuel-coolant structure in the core. Hundreds of thousands of fuel pebbles make full-core Computational Fluid Dynamics (CFD) simulations impractical, while the lack of a natural subchannel precludes simple “hot-channel” type analyses. By averaging the flow equations in space and providing additional closure relationships to approximate the effect of a porous solid matrix of fuel on the coolant, porous media models can provide medium-resolution simulation results with less than 1% the computational cost of detailed CFD models to facilitate accelerated engineering-

scale design and analysis (Ge et al., 2016).

Pronghorn is a Finite Element (FE) porous media PBR Thermal-Hydraulic (T/H) simulation code built on the Multiphysics Object-Oriented Simulation Environment (MOOSE) framework (Gaston et al., 2015) that is intended to predict flow and heat transfer in short turn-around times for design scoping studies and provide core Boundary Conditions (BCs) for systems-level analysis. The extreme ranges in length scales in PBRs, from millimeter-size coated fuel particles to meter-size plant components, necessitates the use of multi-scale T/H techniques. All software built on the MOOSE framework share a common code base, which enables multiphysics coupling and leverages the many domain-specific development hours dedicated to individual-physics codes. Pronghorn provides multiscale T/H capabilities through coupling with the BISON nuclear fuels performance (Hales et al., 2013) and the RELAP-7 (Berry et al., 2014) and SAM (Hu, 2017) systems-level

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T/H codes.

Pronghorn began development in 2008 (Park et al., 2009), but due to recent changes in the MOOSE framework and improved models, was recently redeveloped from scratch. This paper presents an introduction to the models used in Pronghorn and presents validation results of one particular model for all 52 steady-state axisymmetric SANA pebble bed experiments conducted in Germany from 1994–1996 (Stocker and Niessen, 1996). This publication is an extension of previous validation and software development efforts summarized elsewhere (Zou et al., 2018; Novak et al., 2018).

The accuracy of porous media simulations is dependent on the closure relationships used to describe the solid–fluid phase distribution, interphase momentum and energy transfer, and lumped parameter effective heat transfer. The work presented here quantifies the sensitivity of pebble temperature to the porosity, near-wall effective solid thermal conductivity, interphase heat transfer and drag, and thermal dispersion models — the five porous media closures that tend to vary the most between applications to gas-cooled PBRs. In addition, the sensitivity to experimental and material parameters is briefly discussed.

This paper is organized as follows: Section 2 discusses the physical models; Section 3 briefly describes the numerical method; and Section 4 presents an overview of Pronghorn’s verification framework. Section 5 describes the SANA experiments and the modeling assumptions made in the Pronghorn simulations. Section 6 presents baseline results using a single set of closure relationships and comparisons to Flownex and GAMMA, two comparable porous media codes, where available (du Toit et al., 2006; Lim and No, 2006). Eight cases covering most varieties of fluids and pebbles are presented in detail, but for conciseness the remaining 44 cases are only presented as error histograms. One open plenum case is discussed as a separate demonstration of Pronghorn’s simulation capabilities for bed-to-plenum heat and mass transfer. Section 7 explores the sensitivity of pebble temperature to closure selection. Finally, Section 8 provides conclusions on the applicability of Pronghorn’s friction-dominated model to the simulation of gas-cooled PBRs and guidance on closure selection.

2. Physical models

Numerical solutions to the fluid flow equations for nuclear reactor applications are computationally expensive due to the need to resolve boundary layers and capture fine-scale turbulent motions. This cost can be prohibitive to accelerated design and analysis of engineering-scale phenomena such as reactor response to a Loss of Forced Circulation (LOFC) transient. Provided the global impact of local variation in fluid flow and heat transfer can be accurately approximated, a simpler set of equations, the porous media equations, can be solved to predict reactor response. The porous media versions of the governing T/H equations are derived by averaging the equations over a Representative Elementary Volume (REV) consisting of a mixture of solid and fluid (Gray and O’Neill, 1976) characterized by the porosity ϵ , which represents the fraction of the REV that is fluid,

$$\epsilon \equiv \frac{\text{fluid volume}}{\text{total volume}}. \quad (1)$$

Sections 2.1 and 2.2 describe the two flow models available in Pronghorn — the first a compressible Euler model and the second a pseudo-steady friction-dominated model. The remainder of this work then focuses exclusively on the friction-dominated model and its validation with the SANA experiments. Other work has separately focused on verification of the compressible Euler model (Novak et al., 2018). Section 2.3 describes the BCs, Section 2.4 describes the Equation of State (EOS) system, and Section 2.5 describes the closures used in the present work. Note that many additional BCs, material properties, and closures are available in Pronghorn beyond those highlighted here for use in the present analysis; these are described in the theory manual (Novak et al., 2018).

2.1. Compressible Euler model

Pronghorn’s compressible Euler model is derived by averaging the Navier-Stokes equations with conjugate heat transfer in space over a heterogeneous REV. Assuming thermal non-equilibrium between the phases, this equation set includes conservation of fluid mass, momentum, and energy, with conservation of solid energy,

$$\epsilon \frac{\partial \rho_f}{\partial t} + \nabla \cdot (\epsilon \rho_f \vec{V}) = 0, \quad (2)$$

$$\epsilon \frac{\partial (\rho_f \vec{V})}{\partial t} + \nabla \cdot (\epsilon \rho_f \vec{V} \vec{V}) + \epsilon \nabla P - \epsilon \rho_f \vec{g} + W \rho_f \vec{V} = 0, \quad (3)$$

$$\epsilon \frac{\partial (\rho_f E_f)}{\partial t} + \nabla \cdot (\epsilon \rho_f H_f \vec{V}) - \epsilon \rho_f \vec{g} \cdot \vec{V} - \nabla \cdot (\kappa_f \nabla T_f) + \alpha (T_f - T_s) - \dot{q}_f = 0, \quad (4)$$

$$(1 - \epsilon) \rho_s C_p \frac{\partial T_s}{\partial t} - \nabla \cdot (\kappa_s \nabla T_s) + \alpha (T_s - T_f) - \dot{q}_s = 0. \quad (5)$$

Eqs. (2)–(5) are referred to here as the “compressible Euler” model. In Eqs. (2)–(5), f and s subscripts indicate the fluid and solid phases, respectively. $\vec{V}$ is the intrinsic fluid velocity, P is the pressure, T is the phase temperature, and $\vec{g}$ is the gravitational acceleration vector. ρ , E , H , and C_p are the densities, total energies, total enthalpies, and isobaric specific heats, respectively. $\dot{q}$ is a generic volumetric heat source. The viscous shear stress is approximated with a distributed loss friction model due to the many fluid-solid surfaces in a PBR core and the relatively high Reynolds numbers expected in most simulations. This permits simpler BCs and stabilization formulations. The porosity is assumed constant with respect to time because refueling pebble motion occurs on much longer time scales than fluid motion. Eqs. (2)–(5) may be solved for conservative or primitive variables through the application of a change-of-variables low-Mach preconditioner (Hauke and Hughes, 1994).

During the averaging process, several closures arise to capture the momentum and energy transfer between the phases. W is the interphase drag coefficient, κ is the effective thermal conductivity, and α is the interphase heat transfer coefficient. Models for these closures and porosity are described in Section 2.5.

2.2. Friction-dominated model

Pronghorn’s friction-dominated model is derived by setting the total derivative of momentum in Eq. (3) to zero, giving a pseudo-steady momentum equation,

$$\epsilon \nabla P - \epsilon \rho_f \vec{g} + W \rho_f \vec{V} = 0. \quad (6)$$

Eq. (6) is applicable to slowly-evolving, low Reynolds number flows, since momentum conservation is assumed dominated by friction and changes in pressure are instantaneously reflected as changes in momentum. The relative importance of drag relative to momentum advection in low-flow gas-cooled PBRs justifies the use of the friction-dominated model for the SANA experiments (du Toit et al., 2006). Substituting Eq. (6) into Eq. (2) gives a pressure Poisson equation,

$$\epsilon \frac{\partial \rho_f}{\partial t} + \nabla \cdot \frac{\epsilon^2}{W} (-\nabla P + \rho_f \vec{g}) = 0. \quad (7)$$

In addition, a primitive variable formulation of the fluid energy equation is available to simplify the application of BCs,

$$\epsilon \rho_f C_{pf} \frac{\partial T_f}{\partial t} + \epsilon \rho_f C_{pf} \vec{V} \cdot \nabla T_f - \nabla \cdot (\kappa_f \nabla T_f) + \alpha (T_f - T_s) - \dot{q}_f = 0. \quad (8)$$

Eqs. (5)–(8) are referred to here as the “friction-dominated” model, and are very similar to the set of equations solved in a number of other PBR porous media codes (Hossain et al., 2008; Nouri-Borujerdi and Ghomsheh, 2015; IAEA, 2000).

2.3. Boundary conditions

This section describes the BCs available for use with the friction-dominated model. Both Dirichlet and Neumann BCs can be specified. Neumann BCs are additive within the MOOSE framework, permitting modularization. In the discussion that follows, *i* and *o* subscripts indicate known inlet and outlet values and “in,” “out,” and “wall” indicate inflow, outflow, and solid wall boundaries. Γ indicates the boundary with unit outward normal $\hat{n}$ corresponding to a domain with interior Ω . For the pressure Poisson equation in Eq. (7), a Dirichlet value of pressure is specified on the outlet; the corresponding Neumann-type BCs for walls and inlets are

$$\frac{\epsilon^2}{W} (-\nabla P + \rho_f \vec{g}) \cdot \hat{n} = \begin{cases} \rho_f \vec{V}_i \cdot \hat{n} & \Gamma_{\text{in}} \\ 0 & \Gamma_{\text{wall}} \end{cases} \quad (9)$$

No BCs are required for the momentum equation in Eq. (6) provided the pressure gradient is not integrated by parts in the weak form. For the fluid energy equation in Eq. (8), a Dirichlet value for fluid temperature can be specified on any boundary; the corresponding Neumann-type BCs are

$$-\kappa_f \nabla T_f \cdot \hat{n} = \begin{cases} \tilde{q}_f & \Gamma_{\text{known heat flux}} \\ -k_\infty \nabla T_\infty \cdot \hat{n} & \Gamma_{\text{conduction}} \\ h(T_f - T_\infty) & \Gamma_{\text{convection}} \end{cases} \quad (10)$$

where $\tilde{q}_f$ is a known heat flux into the fluid phase; k_∞ is the thermal conductivity of adjacent material; T_∞ is the temperature of adjacent material; and h is the convective heat transfer coefficient. Radiation heat transfer between the fluid and the surroundings is neglected. For the solid energy equation in Eq. (5), a Dirichlet value for solid temperature can be specified on any boundary; the corresponding Neumann-type BCs are

$$-\kappa_s \nabla T_s \cdot \hat{n} = \begin{cases} \tilde{q}_s & \Gamma_{\text{known heat flux}} \\ -k_\infty \nabla T_\infty \cdot \hat{n} & \Gamma_{\text{conduction}} \\ h(T_s - T_\infty) & \Gamma_{\text{convection}} \\ \epsilon \sigma (T_s^4 - T_\infty^4) & \Gamma_{\text{radiation}} \end{cases} \quad (11)$$

where $\tilde{q}_s$ is a known heat flux into the solid phase; ϵ is the emissivity of the solid; and σ is the Stefan–Boltzmann constant.

For steady-state, the thermal resistance concept may be used to approximate series conduction through multiple material layers with a parallel convection and radiation resistance from the surface to the ambient. The heat flux from a boundary may then given as

$$\tilde{q} = \frac{1}{A} \frac{T - T_\infty}{\sum_{i=1}^{n_l} R_{\text{cond},i} + \frac{1}{(h + h_r) A_s}}, \quad (12)$$

where A is the area of the boundary; A_s is the area of the surface; n_l is the number of conduction layers; $R_{\text{cond},i}$ is the conduction resistance of the *i*-th layer; and h_r is the radiation heat transfer coefficient,

$$h_r = \epsilon \sigma (T_{\text{surf}}^2 + T_\infty^2)(T_{\text{surf}}^1 + T_\infty), \quad (13)$$

where T_{surf} is the surface temperature. Iteration is performed to obtain T_{surf} using under-relaxed fixed point iteration. Applying Eq. (12) in 2-D and 3-D systems approximates the heat transfer through the conduction

layers as unidirectional along $\hat{n}$, permitting a simpler mesh.

In some cases, the total value for the heat flux $\tilde{q}_f + \tilde{q}_s$ is known, and without local thermal equilibrium between the phases, an assumption must be made in regard to how this flux is split between the phases. It is assumed that the heat flux is split based on the effective thermal conductivities of the two phases,

$$\tilde{q}_f = \frac{\kappa_f}{\kappa_f + \kappa_s} (\tilde{q}_f + \tilde{q}_s), \quad (14)$$

where the heat flux into the solid phase comprises the remainder of the total heat flux.

2.4. Equations of state

The fluid density, viscosity, thermal conductivity, and specific heat as a function of pressure and temperature are required to close the system. The object-oriented structure of MOOSE allows the use of any of the EOS in RELAP-7 and the fluid properties module. In addition to these properties, helium, nitrogen, FLiBe, and FLiNaK properties are available (Novak et al., 2018). In the present work, helium and nitrogen properties are evaluated based on the most accurate thermophysical data currently available (Ortiz-Vega et al., 2018; Arp et al., 1998; Hands and Arp, 1981; Lemmon and Jacobsen, 2004; Span et al., 2000) using the Spline-Based Table Lookup (SBTL) method (Kunick, 2018).

In addition to the fluid properties, the solid density, thermal conductivity, and specific heat as a function of temperature are required. Graphite, matrix graphite, aluminum oxide, stainless steel, and TRistructural ISOTropic (TRISO) particle layer properties are currently available (Novak et al., 2018). A variety of mixing rules are available to approximate homogenized properties for heterogeneous media. Custom fluid and solid properties may also be defined as temperature-dependent functions in the input file.

2.5. Porous media closure relationships

2.5.1. Porosity

The porosity has an important impact on the flow and heat transfer — all other porous media closures are generally dependent on porosity. The lower the porosity, the higher the drag on the fluid and the greater the convective heat transfer due to the enhanced mixing. Depending on the relative thermal conductivities of the phases, the conduction components of the effective solid thermal conductivity may increase or decrease with porosity, while the larger void spaces associated with higher porosities increase radiation heat transfer (You et al., 2017). The porosity also impacts the local fluid flow area.

The porosity is a function of both the radial and axial distance from bounding walls and free surfaces. The radial dependence of the porosity is a damped, oscillatory function of the distance from the wall, reaching a nearly constant value four to five pebble diameters from the wall (Auwerda et al., 2013; Cohen and Metzner, 1981; du Toit, 2008). The high porosity near the wall results in lower drag and a flow-channeling effect, with a large peak in velocity near the wall (Vortmeyer and Schuster, 1983). This bypass flow results in less effective cooling of the center of the bed, resulting in higher bed temperatures (Auwerda et al., 2011; Becker and Laurien, 2002) and more nonuniform outlet temperatures (Zhao et al., 2010). However, this channeling effect directs more fluid towards the large power peaks observed adjacent to reflectors in thermal-spectrum systems. If the bed to pebble diameter ratio is smaller than approximately 10–30, the overall pressure drop may also be substantially lower than that predicted using a constant porosity (Auwerda et al., 2011; Cohen and Metzner, 1981).

The majority of porous media simulations only consider a radial dependence for porosity (Becker and Laurien, 2002; Becker and Laurien, 2003; du Toit et al., 2006; Lim and No, 2006; Nouri-Borujerdi and Ghomsheh, 2015; IAEA, 2000; Baggemann et al., 2016; Ge et al., 2016), though the axial dependence is also a damped oscillatory

function of the distance from bounding walls, with a smooth approach to unity at free surfaces (Auwerda et al., 2013). Some experimentalists have quantified an axial dependence in a bulk sense (Scott, 1960) or have used discrete element simulations to obtain a fully 3-D profile for a specific system (Auwerda et al., 2011; Suikkanen et al., 2014), but few correlations exist to describe the axial dependence in as general a sense as those describing the radial dependence. Approximately half of the experimental measurements in the SANA facility are taken within two pebbles of the top and bottom boundaries, and neglecting axial effects in the porosity may be significant.

A method for constructing a 2-D r - z porosity profile in terms of two 1-D (radial and axial) porosity profiles is implemented in Pronghorn. The radial dependence of porosity is typically a function of pebble diameter d_p , the minimum distance to a bounding radial wall d_r , the porosity at the wall ϵ_{wall} , and the infinite-medium porosity ϵ_{∞} . This dependence may be expressed as

$$\epsilon(r) = f(d_p, d_r, \epsilon_{\text{wall}}, \epsilon_{\infty}), \quad (15)$$

where f indicates a radial functional dependence. An approximate 2-D profile is obtained by substituting the constant ϵ_{∞} in Eq. (15) with a 1-D axial porosity profile, which is itself a function of the pebble diameter, minimum distance to a bounding axial wall d_z , ϵ_{wall} , and ϵ_{∞} ,

$$\begin{aligned} \epsilon(r, z) &= f(d_p, d_r, \epsilon_{\text{wall}}, \epsilon_{\infty}(z)) \\ &= f(d_p, d_r, \epsilon_{\text{wall}}, g(d_p, d_z, \epsilon_{\text{wall}}, \epsilon_{\infty})), \end{aligned} \quad (16)$$

where g indicates an axial functional dependence. In other words, the infinite-medium porosity used in the radial dependence is computed based on an assumption for the axial dependence. The use of minimum distances to bounding walls assumes that the porosity is independent of the curvature of the walls, which is justified by experimental data (du Toit, 2008). An exponential dependence for porosity is assumed in both the radial and axial directions,

$$\epsilon(r) = \epsilon_{\infty}(z) + \epsilon_{\text{wall}} - \epsilon_{\infty}(z)e^{-6 d_r/d_p}, \quad (17)$$

where $\epsilon_{\infty}(z)$ in Eq. (17) is given as

$$\epsilon_{\infty}(z) = \epsilon_{\infty} + (\epsilon_{\text{wall}} - \epsilon_{\infty})e^{-6 d_z/d_p}. \quad (18)$$

The selection of an exponential profile is motivated by the ability to use a coarser mesh and obtain faster numerical convergence due to the smaller extent of the high-gradient porosity regions than an oscillatory profile. An exponential profile is obtained through the use of larger spatial averaging bins in porosity measurements, so simulation results should be construed as averaged over larger regions in space than when using an oscillatory porosity profile.

The governing T/H equations typically become stiff and difficult to solve in regions where porosity tends to unity (Vortmeyer and Schuster, 1983). To further improve convergence, ϵ_{wall} is set to 0.8, which may also be motivated by apparent decreases in porosity in near-wall regions due to the presence of fluid stagnation points near pebble-wall contact points (Becker and Laurien, 2003; du Toit, 2008). Finally, ϵ_{∞} is dependent on the bed filling method (Scott, 1960), and without specific details regarding the construction of the SANA facility, is left to the discretion of the modeler. In the present study, ϵ_{∞} is set to 0.39.

2.5.2. Drag coefficient

The friction factor W represents the sum of viscous and inertial drag. The Kerntechnischer Ausschuss (KTA) correlation expresses the overall drag as

$$W = 160 \frac{(1 - \epsilon)^2 \mu_f}{\epsilon d_p^2 \rho_f} + 3 \left(\frac{1 - \epsilon}{Re} \right)^{0.1} \frac{(1 - \epsilon) \|\vec{V}\|}{d_p}, \quad (19)$$

where μ_f is the fluid viscosity and Re is the Reynolds number based on the superficial velocity and pebble diameter. Eq. (19) is valid for $1 < Re/(1 - \epsilon) < 10^5$, $0.36 < \epsilon < 0.42$, and d_{bed}/d_p above a limiting curve dependent on the Reynolds number (KTA, 1981). Depending on

the porosity profile and Reynolds number, Eq. (19) may not be applicable. Therefore, a second friction factor correlation developed by Ergun is investigated (Ergun, 1952),

$$W = 150 \frac{(1 - \epsilon)^2 \mu_f}{\epsilon d_p^2 \rho_f} + 1.75 \frac{(1 - \epsilon) \|\vec{V}\|}{d_p}. \quad (20)$$

Pronghorn also includes capabilities for anisotropic drag coefficients, which may be used for modeling of control rod channels and reflector block bypass flows.

2.5.3. Interphase heat transfer coefficient

The interphase heat transfer coefficient α captures convective heat transfer between the phases, and is defined based on the conventional convective heat transfer coefficient multiplied by the wetted heat transfer area per unit length,

$$\alpha = \frac{6(1 - \epsilon) Nu k_f}{d_p}, \quad (21)$$

where Nu is the Nusselt number based on pebble diameter and k is the thermal conductivity. The KTA correlation expresses the convective heat transfer coefficient as

$$Nu = 1.27 \frac{Pr^{1/3} Re^{0.36}}{\epsilon^{1.18}} + 0.033 \frac{Pr^{0.5} Re^{0.86}}{\epsilon^{1.07}}, \quad (22)$$

where Pr is the Prandtl number. Eq. (22) is valid for $100 \leq Re \leq 10^5$ and $0.36 < \epsilon < 0.42$ (KTA, 1983). Depending on the porosity profile and Reynolds number, Eq. (22) may not be applicable. Therefore, a second correlation developed by Gnielinski is investigated,

$$Nu = 1 + 1.5(1 - \epsilon)(2 + \sqrt{Nu_{\text{lam}}^2 + Nu_{\text{turb}}^2}), \quad (23)$$

where Nu_{lam} and Nu_{turb} are the laminar and turbulent Nusselt numbers,

$$Nu_{\text{lam}} = 0.664(Re/\epsilon)^{0.5} Pr^{1/3}, \quad (24)$$

$$Nu_{\text{turb}} = \frac{0.037(Re/\epsilon)^{0.8} Pr}{1 + 2.443(Re/\epsilon)^{-0.1} (Pr^{2/3} - 1)}. \quad (25)$$

Eq. (23) is valid for $Re/\epsilon \leq 7.7 \times 10^5$, $0.7 \leq Pr \leq 10^4$, and $0.26 \leq \epsilon \leq 0.935$ (Achenbach, 1995).

2.5.4. Effective fluid thermal conductivity

The effective fluid thermal conductivity κ_f represents heat transfer enhancement due to additional mixing and recirculation induced by the solid phase, a phenomenon known as “thermal dispersion.” For large Reynolds numbers, heat transfer via thermal dispersion is negligible (Littman et al., 1968), in which case κ_f is given as

$$\kappa_f = \epsilon k_f. \quad (26)$$

Because of the large Reynolds numbers expected, many PBR porous media simulations neglect thermal dispersion (Suikkanen et al., 2014, 2014.; Seker and Downar, 2007; du Toit et al., 2006). For the low Reynolds numbers expected in the SANA facility, however, thermal dispersion may be significant. Thermal dispersion is typically modeled as a linear function of the Peclet number,

$$\kappa_f = \epsilon k_f + C_0 Re Pr k_f, \quad (27)$$

where C_0 is a proportionality coefficient that is typically correlated independently for the radial and axial directions in cylindrical beds (Yagi and Kunii, 1957). For simplicity, an isotropic formulation is used in Pronghorn with $C_0 = 0.11$, similar to other simulations (Auwerda et al., 2011; Becker and Laurien, 2002; Becker and Laurien, 2003). C_0 is halved within a half pebble diameter of the walls to account for wall effects (Tsotsas and Schlünder, 1988).

2.5.5. Effective solid thermal conductivity

The effective solid thermal conductivity κ_s represents three parallel

heat transfer paths that arise because of the porous nature of the medium: 1) conduction in a pebble and radiation between pebbles across a transparent fluid; 2) conduction in a pebble and conduction in the fluid between pebbles; and 3) conduction in a pebble and conduction between pebbles at contact areas. These three components are denoted as $\kappa_{\text{radiation}}$, $\kappa_{\text{conduction}}$, and κ_{contact} , respectively, and κ_s is the sum of these heat transfer modes,

$$\kappa_s = \kappa_{\text{radiation}} + \kappa_{\text{conduction}} + \kappa_{\text{contact}}. \quad (28)$$

The Breitbach and Barthels correlation is used for $\kappa_{\text{radiation}}$,

$$\kappa_{\text{radiation}} = (1 - \sqrt{1 - \epsilon}) \epsilon + \frac{\sqrt{1 - \epsilon}}{2/\epsilon - 1} \frac{B + 1}{B} \frac{1}{1 + \frac{4\sigma T^3 d_p}{(2/\epsilon - 1)\kappa_s}} 4\sigma d_p T^3, \quad (29)$$

where B is given as

$$B = 1.25 \left(\frac{1 - \epsilon}{\epsilon} \right)^{10/9}, \quad (30)$$

and T is the bed average temperature, assumed to be the local solid temperature (Auwerda et al., 2011; Breitbach and Barthels, 1979).

The Zehner and Schlünder model is used for $\kappa_{\text{conduction}}$ (Tsotsas and Martin, 1987),

$$\kappa_{\text{fluidconduction}} = (1 - \sqrt{1 - \epsilon}) k_f + \sqrt{1 - \epsilon} \mathcal{K}_{SF} k_f, \quad (31)$$

where $\mathcal{K}_{SF}$ is given as

$$\mathcal{K}_{SF} = \frac{2}{1 - B\lambda} \frac{B(1 - \lambda)}{(1 - B\lambda)^2} \ln\left(\frac{B}{\lambda}\right) - \frac{B - 1}{1 - B\lambda} - \frac{B + 1}{2}, \quad (32)$$

and λ is the fluid-to-solid thermal conductivity ratio,

$$\lambda = \frac{k_f}{k_s}. \quad (33)$$

Finally, the Chan and Tien model is used for κ_{contact} (Chan and Tien, 1973),

$$\kappa_{\text{contact}} = \frac{1}{2 \cdot 0.53} \frac{N_A}{N_L} \left(\frac{d_c}{d_p} \right) d_p k_s, \quad (34)$$

where N_A and N_L are the number of spheres per unit area and length, respectively, in the unit cell; and d_c is the diameter of the contact area between touching spheres. The contact diameter is estimated from Hertzian elastic deformation theory as (You et al., 2017)

$$\frac{d_c}{d_p} = \left(\frac{3}{4} \frac{1 - \nu_p^2}{E} \frac{4F}{d_p^2} \right)^{1/3}, \quad (35)$$

where ν_p is the Poisson ratio of the solid, E is the elastic modulus of the solid, and F is the collinear force between pebbles,

$$F = S_F \frac{P}{N_A}, \quad (36)$$

where S_F is a factor that relates the total force to the vertical component, assumed to be the pressure P due to pebble weight. The pressure is approximated as

$$P(z) = (1 - \epsilon_\infty) \rho_s \bar{V}(z) |g_z|, \quad (37)$$

where $\bar{V}(z)$ is the volume of the bed above elevation z and $|g_z|$ is the magnitude of the axial component of the gravitational acceleration. Interpolation is performed between ordered lattice N_A , N_L , and S_F values.

Most correlations are only applicable within the bulk region of the bed. For example, Eq. (29) tends to infinity as porosity tends to unity, a nonphysical trend. Within a half pebble diameter of the walls, better agreement with experimental data is obtained by either using a different set of correlations altogether (Auwerda et al., 2011) or through application of a multiplicative constant (IAEA, 2000). Two approaches

are investigated here — applying a multiplier of 0.5 to κ_s or using the Tsotsas correlation for $\kappa_{\text{radiation}}$ (Visser, 2007),

$$\kappa_{\text{radiation}} = (1 - \sqrt{1 - \epsilon}) \frac{4\sigma T^3 d_p}{k_f (2\epsilon - 1)} + \sqrt{1 - \epsilon} \left(\frac{k_f (2\epsilon - 1)}{4\sigma T^3 d_p} + \lambda \right)^{-1}. \quad (38)$$

To obtain continuity with the bulk value of $\kappa_{\text{radiation}}$, the minimum of Eqs. (29) and (38) is used in the near-wall region.

3. Numerical method

Pronghorn is based on the Finite Element Method (FEM); discretized forms of Eqs. (5)–(8) are obtained by multiplying the strong residuals by a weight function ψ , integrating over the domain Ω , and applying integration by parts where possible,

$$\int_{\Omega} \left(\epsilon \frac{\partial P}{\partial x_j} - \epsilon \rho_f g_j + W \rho_f V_j \right) \psi \, d\Omega = 0, \quad (39)$$

$$\int_{\Omega} \epsilon \frac{\partial \rho_f}{\partial t} \psi \, d\Omega + \int_{\Omega} \frac{\epsilon^2}{W} (\nabla P - \rho_f \vec{g}) \cdot \nabla \psi \, d\Omega - \int_{\Gamma} \frac{\epsilon^2}{W} (\nabla P - \rho_f \vec{g}) \cdot \hat{n} \psi \, d\Gamma = 0, \quad (40)$$

$$\int_{\Omega} \epsilon \rho_f C_{pf} \frac{\partial T_f}{\partial t} + \epsilon \rho_f C_{pf} \vec{V} \cdot \nabla T_f + \alpha \left(T_f - T_s \right) - \dot{q}_f \psi \, d\Omega + \int_{\Omega} \kappa_f \nabla T_f \cdot \nabla \psi \, d\Omega - \int_{\Gamma} \kappa_f \nabla T_f \cdot \hat{n} \psi \, d\Gamma = 0, \quad (41)$$

$$\int_{\Omega} \left(1 - \epsilon \right) \rho_s C_{ps} \frac{\partial T_s}{\partial t} + \alpha \left(T_s - T_f \right) - \dot{q}_s \psi \, d\Omega + \int_{\Omega} \kappa_s \nabla T_s \cdot \nabla \psi \, d\Omega - \int_{\Gamma} \kappa_s \nabla T_s \cdot \hat{n} \psi \, d\Gamma = 0, \quad (42)$$

where j subscripts in Eq. (39) indicate the j -th momentum equation. The objective of the FEM is to find a solution $u \in H^1(\Omega)$ such that $u|_{\Gamma_u} = U$ and $\psi \in H^1(\Omega)$ such that $\psi|_{\Gamma_u} = 0$. $H^1(\Omega)$ is the Hilbert-space norm ensuring finite first derivatives and Γ_u is the portion of the boundary with Dirichlet BCs U .

It is well-known that the Galerkin FEM, in which the solution is in the same function space as the weight functions, is conditionally unstable when applied to convection–diffusion equations (Hughes et al., 2010). The Streamline-Upwind Petrov-Galerkin (SUPG) method is implemented in Pronghorn for both the compressible Euler and friction-dominated models to overcome such instabilities (Novak et al., 2018).

After spatial discretization, the Jacobian-Free Newton Krylov (JFNK) method is used to solve the system of coupled nonlinear equations. This solution method uses an outer loop over Newton iterations and an inner loop over linear iterations. The Jacobian required for the Newton iterations is approximated with a first-order accurate finite difference derivative. Linear iterations are performed using the Generalized Minimal Residuals (GMRES) method. Method of lines temporal discretization is used for time discretization with implicit timestepping. All MOOSE applications are automatically parallel with hybrid Message Passing Interface (MPI) and OpenMP parallelism.

4. Code verification

All models in Pronghorn are subject to a rigorous verification and testing framework. All physics kernels and BCs must show theoretical convergence rates using the Method of Manufactured Solutions (MMS) combined with mesh and/or timestep refinement studies. Unit tests are used to ensure correct closure models and fluid and solid property implementations.

For illustration, the convergence rates calculated using the L^2 norm of the FE error based on MMS tests are shown in Fig. 1 for (a) the $-\nabla \cdot (\kappa_s \nabla T_s)$ kernel and (b) the $\epsilon \rho_f C_{pf} \partial T_f / \partial t$ kernel. The expected

Fig. 1. MMS convergence studies for (a) the $\nabla \cdot (\kappa_s \nabla T_s)$ kernel; and (b) the $\epsilon \rho_f C_{p_f} \partial T_f / \partial t$ kernel. “BDF 2” and “DIRK” represent Backward Differentiation Formula 2 and Diagonally-Implicit Runge-Kutta, respectively. Discrete points are error measurements and solid lines are linear fits.

convergence rates of 2 and 3 for linear and quadratic elements, respectively, are obtained for the spatial kernel. The expected convergence rates of 1 or 2 are obtained for various time discretization schemes for the time-dependent kernel.

5. The SANA facility and Pronghorn model

The SANA facility consists of a cylindrical steel vessel containing about 9500 non-fueled spheres, with either helium or nitrogen coolant and either 6 cm electric graphite pebbles, 3 cm matrix graphite pebbles, or 6.5 cm aluminum oxide pebbles. A depiction of the facility is given in Fig. 2. The bed is heated by between one and four electrical resistance heater elements. The pebble temperature is measured throughout the bed with thermocouples. Insulation is present on the bottom and top of the bed to limit axial heat loss. The maximum power density of 28 kW/m³ corresponds to 0.93% of the full power of a typical gas-cooled PBR design, or decay heat levels several hours after shutdown. Both steady-state and transient tests were completed with either a single heater in the center of the bed in an axisymmetric layout or with multiple heaters placed throughout the bed. In some cases, heating is only applied in the

bottom half or top half of the bed.

The present work focuses on simulation of all 52 axisymmetric steady-state cases. The validation results for eight cases are presented in detail, while the remaining 44 are summarized with error histogram plots for brevity. These eight cases were selected to cover most of the range of powers, heater arrangements, coolants, and pebble types used in the experiments, in addition to permitting direct comparison with available Flownex and GAMMA results. Fluid temperature and velocity results, for which no experimental data exists, are shown for a number of additional experiments aside from the eight highlighted cases. Table 1 summarizes these eight cases, plus one open plenum case, and provides case letters for differentiation.

Because no significant azimuthal asymmetries exist, the present analysis uses a 2-D cylindrically-symmetric mesh. However, Pronghorn can in general run on 3-D unstructured meshes. For simplicity, only the interior of the vessel is modeled. The effects of insulation and the vessel are accounted for using the thermal resistance BC in Eq. (12) applied to the solid energy equation. Due to the lower thermal conductivity of the fluid phase and the low velocities expected, the fluid is assumed insulated on all boundaries except the heater surface. The heat flux is assumed uniform along the surface of the heater and is split between the phases according to Eq. (14). Zero normal mass flux is weakly imposed on all surfaces, while tangential slip is permitted. On the surface of the vessel, a combined convection and radiation condition is applied assuming a steel emissivity of 0.8 and a constant convection coefficient of 15 W/m²K. As insufficient data is provided with the benchmark information, the natural convection coefficient is selected arbitrarily to be within the range of 5–25 W/m²K used by other participants (Rousseau

Fig. 2. Illustration of the SANA facility with a single full-height central heater (Stocker and Niessen, 1996).

Table 1

A summary of the SANA cases simulated with Pronghorn, with case letters for reference.

Case	Heater description	Pebble Type	d_p (cm)	Fluid	Power (kW)
A	Full-height	Graphite	6.0	He	5
B	Full-height	Graphite	6.0	He	35
C	Full-height	Graphite	6.0	N	5
D	Full-height	Graphite	6.0	N	35
E	Full-height	Aluminum oxide	6.5	He	30
F	Full-height	Aluminum oxide	6.5	N	30
G	Bottom half	Graphite	6.0	He	20
H	Bottom half	Graphite	6.0	N	20
I	Bottom half, open plenum	Graphite	6.0	N	5

et al., 2006; Baggemann et al., 2016; Becker and Laurien, 2003; Lim and No, 2006; IAEA, 2000). The heat flux is assumed uniform along the surface of the heater. The pebble emissivity, elastic modulus, and Poisson ratio are not provided in the benchmark documentation, so are assumed to be 0.8, 9×10^9 Pa, and 0.136, respectively, for all pebbles (Stocker and Niessen, 1996).

Section 7 presents an analysis of the sensitivity of solid temperature to different closure models. Before presenting this analysis, Section 6 provides baseline Pronghorn results assuming porosity is given by Eq. (17); the drag coefficient is given by Eq. (19); the interphase heat transfer coefficient is given by Eq. (22); the effective fluid thermal conductivity is given by Eq. (26); and the effective solid thermal conductivity is given by the sum of Eqs. (29), (31), and (34), with Eq. (38) applied in the near-wall region. For the open plenum case, the porosity in the plenum is set to unity, and in the bed is given by Eq. (17) with ϵ_{wall} set to unity to ensure a smooth transition to the plenum.

All cases are run as transients, terminating once the relative change in the solution norm from the previous time step is less than 10^{-6} . Mesh refinement studies are performed for the highest-powered cases of each category of experiment (such as nitrogen coolant with 3 cm pebbles) to verify converged results.

6. Pronghorn SANA results

Pronghorn simulation results for the SANA cases in Table 1, along with code-to-code comparisons where available, are presented in this section. All experimental data are shown as discrete points. Pronghorn results are shown as solid lines, Flownex results are shown as dashed lines, and GAMMA results are shown as dotted lines. Measurements were taken at five axial elevations measured relative to the bottom of the bed; only three of these elevations are plotted to simplify data presentation. An assessment of the modeling errors is provided for all cases at the end of Section 6.1.

Figs. 3 and 4 show Pronghorn and Flownex simulation results for heater powers of 5 and 35 kW and 6 cm graphite pebbles with helium or nitrogen coolant, respectively. The lower thermal conductivity of nitrogen results in a greater fraction of heat transported by convection than conduction, resulting in larger axial temperature gradients compared to helium. Pronghorn and Flownex agree well for the helium cases and reasonably well for the nitrogen cases. Both Pronghorn and Flownex tend to overpredict temperatures near the surface of the heater. Pronghorn predicts lower temperatures at the lowest elevation for the nitrogen cases than Flownex.

Fig. 5 shows Pronghorn simulation results for a heater power of 30 kW and 6.5 cm aluminum oxide pebbles with helium or nitrogen coolant. Compared to the graphite pebble simulations in Figs. 3 and 4, the lower thermal conductivity of the aluminum oxide results in larger

axial temperature gradients and higher predicted peak temperatures by about 400 °C. Pronghorn predicts the experimental data well at all points except at the lowest elevation close to the heater surface for helium.

Fig. 6 shows the fluid temperature for a 30 kW heater power for helium (top row) or nitrogen (bottom row) coolant and the three different types of pebbles. Velocity streamlines are shown as black lines. The rotational symmetry axis is indicated with dashed black lines and arrows. The aluminum oxide pebble results correspond to cases E and F, while the other results correspond to experiments not included in Table 1. The natural circulation flow is visible, with a stagnation point near the outer edge of the bed. The primarily radial diffusion heat transfer in the helium cases results in stagnation points nearer to the axial centerline of the bed than in the convection-dominated, lower viscosity, nitrogen cases. Both graphite pebbles have higher thermal conductivity than the aluminum oxide pebbles, which results in lower peak temperatures.

No experimental data is available for velocities or fluid temperature, but the results in Fig. 6 display the expected physical trends and agree qualitatively with Flownex predictions (du Toit et al., 2006). For case B, not shown in Fig. 6, Pronghorn predicts a helium temperature range of 254–1086 °C, which agrees well with the helium temperature range for the same case predicted by CFX of 284–1085 °C (Becker and Laurien, 2003).

Fig. 7 shows Pronghorn simulation results for a heater power of 20 kW in the bottom half of the bed with 6 cm graphite pebbles and helium or nitrogen coolant. Near the heater surface, the temperature distribution is inverted relative to the long central heater cases in Figs. 3 and 4, being highest at the bottom of the bed. This occurs due to the absence of a heat source in the top of the bed. The lower thermal conductivity of nitrogen results in poorer radial heat transport than in helium, resulting in an opposite temperature trend near the bed periphery compared to helium. Pronghorn tends to underpredict temperatures in the higher elevations relative to Flownex and GAMMA. All codes show similar trends in Fig. 7, but the absolute variation is larger than for the full-length heater results. This may be due to differences in thermal BCs at the heater surface and/or equation models, since the 20 kW half-heater cases represent some of the highest local heat fluxes of the experiments.

Finally, Fig. 8(a) shows Pronghorn simulation results in comparison to experimentally-measured temperatures for a heater power of 5 kW in the bottom half of the bed and an open gas plenum in the top third of the bed for 6 cm graphite pebbles and nitrogen coolant. Fig. 8(b) shows the velocity streamlines as black lines, with the background colored with fluid temperature. Pronghorn solid temperature predictions agree reasonably well with the experimental data, though temperatures are slightly overpredicted near the heater surface at the middle and top

Fig. 3. Pronghorn (—) and Flownex (---) predicted solid temperature for (a) case A and (b) case B.

Fig. 4. Pronghorn (—) and Flownex (---) predicted solid temperature for (a) case C and (b) case D.

elevations. The transition from the pebble bed to the open plenum is clearly visible in the velocity streamlines. Fluid re-entering the porous region is pulled towards the high-porosity region near the wall where drag effects are lower which, when combined with the significantly reduced friction in the open plenum relative to the bed, results in primarily radial flow in the plenum.

It should be noted that the use of a friction-dominated model in the plenum is not justified as in the pebble bed due to the large mixing region present. The accuracy of the Pronghorn solution in the plenum cannot be directly assessed because of a lack of experimental data. Additional validation is required for Pronghorn application to open plenum geometries, even though the solution in the bed region agrees well with experimental data.

6.1. All steady-state axisymmetric tests

This section summarizes the results for all 52 steady-state axisymmetric experiments, giving a total of 1292 experimental pebble temperature data points. For simplicity, the plenum test is excluded from the histograms shown in this section and in Section 7. The error is defined as

$$\text{error} = T_s(\vec{x}_i) - T_{s,\text{exp},i}, \quad (43)$$

where $T_s(\vec{x}_i)$ is the predicted solid temperature at position $\vec{x}_i$ and $T_{s,\text{exp},i}$ is the experimentally-measured solid temperature at position $\vec{x}_i$. The maximum error occurs at the data point with error furthest from zero, and may be either positive or negative. Fig. 9 shows a histogram of the error for all 52 Pronghorn cases, in comparison with histograms for the

available Flownex and GAMMA data. The presentation of the error and standard deviation for all 52 SANA cases together should not be taken as an indication of the expected accuracy of Pronghorn for all applications. Rather, this condensation is performed to provide a quantitative comparison against Flownex and GAMMA and to provide a rough sense of the accuracy of porous media T/H simulations in friction-dominated flows such as LOFC decay heat removal.

Significantly more cases were simulated with Pronghorn than with Flownex and GAMMA. To provide a fair comparison of the average error and standard deviation, Table 2 shows the mean, standard deviation, and maximum error for all 52 cases, the six Flownex cases, and the four GAMMA cases. In each column, the number of points compared between the three tools are the same. When considering only the subset of the Flownex and GAMMA cases, Pronghorn predicts a slightly smaller mean error and lower standard deviation relative to both Flownex and GAMMA. Pronghorn predicts a significantly smaller maximum error for the Flownex cases, but a slightly larger error for the GAMMA cases. Given the cases simulated, the three codes are of comparable accuracy.

The standard deviation for all simulation tools is similar, on the order of 50 °C. The SANA experiments represent a challenging benchmark because of the large thermal gradients near the heater and outer radial wall. Fig. 10 shows the error in the Pronghorn calculations as a function of distance from the radial and axial walls. Black dots represent individual data points, while larger red dots are the means of the data at each value of the independent variable, either the radial distance or the axial distance. The spread, or standard deviation, in the error decreases with distance from radial and axial walls. This is expected because of the isotropic assumptions made in the porous media

Fig. 5. Pronghorn (—) predicted solid temperature for (a) case E and (b) case F.

Fig. 6. Pronghorn predicted velocity streamlines, background colored with fluid temperature, for a 30 kW heater power for helium (top row) or nitrogen (bottom row) coolant for the three different types of pebbles.

closures and the use of closures typically determined from bed-averaged data. Additional contributors to near-wall errors include the use of simplified thermal resistance BCs and momentum equations that permit slip, the latter of which results in an overprediction of the velocity near the wall and a corresponding overprediction of convective heat transfer and drag. Therefore, the large standard deviation of 50 °C can be partially attributed to the significant fraction of experimental data points close to bounding walls. Future work will incorporate a Brinkman viscous stress model in Pronghorn, which will allow quantification of slip-related errors in the near wall regions.

Fig. 10(a) shows that the mean error decreases with distance from the radial walls, while no such trend is clearly visible in Fig. 10(b) for the mean error as a function of distance from the axial walls. This supports the claim that the SANA experiments are a challenging benchmark due to the very large thermal gradients in the radial

direction, as no such decrease in average error exists for distances from the axial walls, which are insulated to the extent that thermal boundary effects are less significant but are still characterized by anisotropic momentum and heat transfer and slip effects. This suggests that 1) the average error in Pronghorn simulations will be lower for systems with less significant thermal boundary layers; and 2) more sophisticated heat flux BCs can potentially reduce mean error in the near-wall regions.

On average, Pronghorn overpredicts the solid temperature by 22.6 °C. In addition to the identified near-wall error contributions of isotropic closures, slip, and simplified resistance BCs, additional modeling approximations that may have affected the accuracy of the simulations include 1) the constant vessel surface convection coefficient and emissivity; and 2) the constant pebble emissivity, elastic modulus, and Poisson ratio. In the long central heater cases shown in Figs. 3–5, temperatures are generally overpredicted near the heater surface. This

Fig. 7. Pronghorn (—), Flownex (---), and GAMMA (···) predicted solid temperature for (a) case G and (b) case H.

Fig. 8. Pronghorn predicted (a) solid temperature and (b) velocity streamlines with background colored with fluid temperature for case I.

Fig. 9. Solid temperature error for Pronghorn (52 cases), Flownex (six cases), and GAMMA (four cases).

may indicate that the closures used for κ_s underpredict the effective thermal conductivity in this region or that the pebble emissivity is too low. Pebble emissivities of 0.9 and 0.85 have been used in similar simulations (IAEA, 2000; IAEA, 2013). Therefore, a higher emissivity is not without precedent, but an emissivity of 0.8 is used in Pronghorn for easier comparison to Flownex and GAMMA.

Additional insight can be obtained when considering the error for different subsets of the experiments as summarized in Table 3. On average, Pronghorn predicts the helium cases with 16.6 °C lower standard deviation than the nitrogen cases. The greater convective transport in nitrogen is more difficult to capture with the friction-dominated model. Pronghorn predicts cases with the two types of graphite pebbles with nearly the same standard deviation, while the aluminum oxide

cases have a higher standard deviation. This may be attributed to the use of graphite emissivity, Young's modulus, and Poisson ratio for the aluminum oxide pebbles due to a lack of aluminum oxide data. The 6 cm graphite pebble cases are predicted with remarkably lower mean error than the other two types of pebbles, which may be partially attributed to the fact that partial-length heater cases were only performed with the 6 cm graphite pebbles. In addition, the KTA correlations for drag and heat transfer were developed based on experiments using 6 cm graphite pebbles. Lower errors for the 3 cm matrix graphite and 6.5 cm aluminum oxide pebbles might be obtained if using closures based on those specific pebble designs.

No experimental data points are used to assign Dirichlet-type BCs as in other simulations (IAEA, 2000; du Toit et al., 2006). The exclusive use of flux BCs better assesses the usage of Pronghorn for prediction of unknown systems where temperature data is not known a priori. Finally, a margin of 1% in temperature, 2 cm in axial position, and 1 cm in radial position introduces some uncertainty in the experimental measurements themselves (Becker and Laurien, 2003).

Overall, a good agreement is obtained with both Flownex and GAMMA. Graphical comparisons against THERMIX, TINTE, and TRIO-EF, not shown in this work, also show good agreement with Pronghorn (IAEA, 2000). Differences between Pronghorn, Flownex, and GAMMA exist due to the use of different closures, equation models, and BCs. For example, neither Flownex nor GAMMA consider an axial dependence in the porosity, while Pronghorn considers a 2-D r - z dependence. Flownex and GAMMA include a viscous stress term in the conservation of momentum equation, while Pronghorn permits slip. Flownex uses a constraint-style equation to represent heat transfer between pebbles, while Pronghorn and GAMMA combine the solid effective heat transfer term with the conservation of solid energy equation. Different vessel surface convection coefficients are used in all three codes. Development efforts in all three applications are required to fully disentangle these simultaneous effects to identify the most significant contributors to the different temperature predictions.

Table 2

The mean, standard deviation, and maximum error for the Flownex cases (A, B, C, D, H, and the 20 kW top half heater with 6 cm graphite pebbles with nitrogen test); GAMMA cases (G, H, and the 30 kW long central heater with 6 cm graphite pebbles with helium and nitrogen tests); and all 52 cases. All units are °C. “—” indicates that data is not available for that subset of cases.

Code	Flownex cases (6)			GAMMA cases (4)			All cases (52)		
	Mean	σ	Max	Mean	σ	Max	Mean	σ	Max
Flownex	19.8	51.4	207.0	—	—	—	—	—	—
GAMMA	—	—	—	−4.3	50.9	147.5	—	—	—
Pronghorn	−7.8	47.5	−155.8	−1.6	48.7	148.4	22.6	54.6	198.6

Fig. 10. Solid temperature error as a function of distance from (a) a radial wall (inner or outer), and (b) an axial wall (lower or upper). Each black dot is one data point. Each red dot is the mean of the error for the data at each value of the independent variable (radial or axial wall distance).

Table 3

The mean, standard deviation, and maximum error for different subsets of the 52 SANA cases.

Subset Description	# Cases	Mean (°C)	σ (°C)	Max (°C)
All cases	52	22.6	54.6	198.6
Helium coolant	26	20.5	45.8	166.7
Nitrogen coolant	26	24.8	62.4	198.6
3 cm matrix graphite pebbles	12	44.2	48.7	198.6
6 cm electric graphite pebbles	28	02.0	48.4	−189.6
6.5 cm aluminum oxide pebbles	12	45.8	55.8	181.3
Full-length heater	36	30.5	52.7	198.6
Partial-length heater	16	03.9	54.7	−189.6

7. Pebble temperature sensitivity to closure relationship selection

This section explores the sensitivity of pebble temperature to particular closure relationships selected for porosity, the near-wall treatment for the solid effective thermal conductivity, interphase heat transfer and drag, and thermal dispersion. This investigation is performed by varying a single closure from the baseline model described in Section 5 and simulating all 52 experiments. All BCs described in Section 5 are unchanged.

Table 4 shows the mean, standard deviation, and maximum error for the baseline Pronghorn model in comparison to various closure modifications. The data in each row was obtained by simulating all 52 cases. For example, the entry labeled “constant porosity” represents simulation results with the porosity closure used in the baseline model replaced by a constant porosity, and so forth. To quantify the

significance of the lack of complete experimental facility information, simulations are also performed for two different constant values of the vessel convection coefficient and for two different values of the pebble emissivity. Results are presented in terms of the thermocouple locations within the bed to illustrate how the error varies as a function of position. The near-wall region is defined to occur within a half pebble diameter of the walls, while the bulk region constitutes all other points. For the baseline model and all closure variations, the mean error and standard deviation are both approximately 10 °C higher in the near-wall region than in the bulk.

Less than 2 °C difference in both the mean and standard deviation are observed when varying the drag, interphase heat transfer, and thermal dispersion models. This relative insensitivity to the drag and heat transfer correlation agrees with results observed by others (Becker and Laurien, 2002).

The solid temperature is sensitive to both the porosity model and the near-wall effective solid thermal conductivity treatment. A constant porosity on average results in a 11.6 °C higher error and a 11.4 °C higher standard deviation than a 2-D porosity. A simple scaling factor applied to the effective solid thermal conductivity in the near-wall region results in a 12.9 °C higher error, but a 2.6 °C lower standard deviation, than the use of a different $\kappa_{\text{radiation}}$ correlation. While a constant porosity only differs from the 2-D r - z porosity in the near-wall region, and the wall treatment for solid effective thermal conductivity is only applied in the near-wall region, it is important to note that the use of these different closures affects the accuracy in all regions of the bed. Additional investigations are required to determine how these conclusions extend to geometries with larger bed to pebble diameter ratios.

Table 4

The mean, standard deviation, and maximum solid temperature error for all 52 cases simulated with Pronghorn as a function of location within the bed for various closure modifications to the baseline model described in Section 5. 459 points occur in the near-wall region; the remaining 833 are in the bulk. All units are °C.

Model	All			Near-Wall			Bulk		
	Mean	σ	Max	Mean	σ	Max	Mean	σ	Max
Baseline	22.6	54.6	198.6	29.3	60.5	198.6	18.9	50.7	181.3
Constant ϵ	34.2	66.0	280.1	42.1	74.4	280.1	29.8	60.4	250.4
Near-wall scaling κ_s	35.5	52.0	197.3	41.3	58.5	197.3	32.3	47.8	191.1
Ergun W	21.1	54.4	211.6	27.2	59.7	−197.8	17.7	50.9	211.6
Gnielinski α	22.0	54.9	211.1	28.2	60.3	−196.3	18.6	51.4	211.1
With dispersion	21.5	54.2	208.1	27.5	59.6	194.1	18.1	50.7	208.1
$h = 10 \text{ W/m}^2\text{K}$	36.1	51.3	218.0	41.4	57.0	206.8	33.2	47.6	218.0
$h = 20 \text{ W/m}^2\text{K}$	11.6	57.8	−215.3	18.5	63.1	−215.3	7.8	54.3	203.6
$\epsilon = 0.7$	35.5	63.6	221.4	45.0	70.7	221.4	30.3	58.7	195.0
$\epsilon = 0.9$	9.5	48.8	−179.5	13.7	53.9	−179.5	7.2	45.7	167.3

The solid temperature is also sensitive to the vessel convection coefficient and pebble emissivity. A range of 24.5 °C in error and 6.5 °C in standard deviation is observed depending on the selection of h , while a range of 26.0 °C in error and 14.8 °C in standard deviation is observed depending on the selection of ϵ . For all the variations in closure parameters, increasing the pebble emissivity from 0.8 to 0.9 is the only change that simultaneously results in a lower mean error, a smaller standard deviation, and a lower maximum error relative to the baseline model. This strong dependence on emissivity has been observed elsewhere, and motivates complete characterization of pebble material properties (IAEA, 2000). Some error and spread in the Pronghorn simulations must therefore be attributed to a lack of complete experimental and material details in the benchmark specifications.

8. Conclusions

At the expense of approximating local flow and heat transfer effects, porous media models can provide medium-fidelity predictions of PBR T/H characteristics to accelerate design and analysis. This paper presented a new porous media thermal-hydraulics simulation code, Pronghorn. Essential to the development of any new simulation tool is the establishment of a strong validation base. Validation of Pronghorn's friction-dominated model with the SANA experiments is illustrated through good agreement with both experimental measurements and comparable tools. Pronghorn predicts lower average error and standard deviation in comparison to Flownex and GAMMA. On average, Pronghorn overpredicts solid temperature by 22.6 °C with a standard deviation of 54.6 °C. The friction-dominated model better predicts the helium cases than the nitrogen cases, suggesting better applicability to systems with greater diffusive effects. Solid temperature predictions are more accurate with lower standard deviation in the bulk region of the bed, which is likely caused by the use of isotropic porous media closures, slip, and simplified thermal resistance BCs.

Statistical analysis shows that the interphase drag, heat transfer, and thermal dispersion models are of little significance to solid temperature. The solid temperature is sensitive to the models used for porosity and the near-wall treatment of the solid effective thermal conductivity in the entirety of the bed. These conclusions only apply to friction-dominated, thermally-driven systems such as the SANA facility for the particular correlations investigated. Finally, the selection of the vessel surface convection coefficient and the pebble emissivity has a significant impact on solid temperature. This motivates careful experimental facility documentation for future benchmarking.

Future work involving the inclusion of more sophisticated modeling capabilities, such as drag and heat transfer correlations applicable to prismatic geometries, a Brinkman viscous term, and a low Mach number model for faster simulation of nearly incompressible fluids, have been outlined with the goals of permitting widespread use of Pronghorn as a fast and accurate thermal-hydraulics simulator for pebble bed and prismatic reactors.

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