A Bayesian Approach for Statistical–Physical Bulk Parameterization of Rain Microphysics. Part I: Scheme Description

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ABSTRACT

A new framework is proposed for the bulk parameterization of rain microphysics: the Bayesian Observationally Constrained Statistical–Physical Scheme (BOSS). It is designed to facilitate direct constraint by observations using Bayesian inference. BOSS combines existing process-level microphysical knowledge with flexible process rate formulations and parameters constrained by observations within a Bayesian framework. Using a raindrop size distribution (DSD) normalization method that relates DSD moments to one another via generalized power series, generalized multivariate power expressions are derived for the microphysical process rates as functions of a set of prognostic DSD moments. The scheme is flexible and can utilize any number and combination of prognostic moments and any number of terms in the process rate formulations. This means that both uncertainty in parameter values and structural uncertainty associated with the process rate formulations can be investigated systematically, which is not possible using traditional schemes. In this paper, BOSS is compared to two- and three-moment versions of a traditional bulk rain microphysics scheme (denoted as MORR). It is shown that some process formulations in MORR are analytically equivalent to the generalized power expressions in BOSS using one or two terms, while others are not. BOSS is able to replicate the behavior of MORR in idealized one-dimensional rainshaft tests, but with a much more flexible and systematic design. Part II of this study describes the application of BOSS to derive rain microphysical process rates and posterior parameter distributions in Bayesian experiments using Markov chain Monte Carlo sampling constrained by synthetic observations.

1. Introduction

The representation of microphysics is a key component of weather and climate models, affecting surface precipitation, latent heating and cooling, cloud radiative properties, and cloud chemistry. However, its parameterization in current models is uncertain, to a large degree. Because there is limited theoretical understanding of most microphysical processes, cloud and precipitation observations are essential for developing and improving microphysics schemes. Moreover, microphysical processes inherently operate at scales several orders of magnitude smaller than can be resolved by even the highest-resolution cloud, weather, and climate models. Schemes must therefore statistically describe the effects of these unresolved processes in models—in essence the classical “parameterization problem”—and for microphysics this is largely guided by observations given the limited theoretical knowledge. This is especially true for
bulk schemes that do not explicitly resolve the drop size distribution (DSD), though bin schemes that explicitly resolve the DSD and Lagrangian schemes that represent the hydrometeor population with a sampling of point particles must still rely heavily on empirical parameters to calculate process rates (e.g., for collection and breakup efficiencies). Borrowing terminology from Schneider et al. (2017), microphysics is dominated by “noncomputable” parameters, as opposed to “computable” parameters associated with known governing equations. Stated simply, there is no benchmark for microphysics parameterization because there is no known complete set of governing microphysical equations. This is distinctly unlike, for example, the Navier–Stokes equation for fluid motion and turbulence. Thus, theoretical constraints for microphysics are primarily integral, that is, conservation of water and energy during phase transitions and positive definiteness of cloud quantities, with limited theoretical constraint of many of the individual processes themselves.

Directly observing microphysical process rates is extremely challenging, especially in natural clouds. There is a wealth of cloud and precipitation observations now available from radar, satellite, and other platforms, but these measure properties that evolve through the net effect of various microphysical and dynamical processes rather than the process rates themselves. For bulk schemes, some studies have formulated processes directly from fitting to process rates modeled by bin schemes over a range of conditions (e.g., Khairoutdinov and Kogan 2000; Chen and Liu 2004; Seifert 2008; Kogan and Belochitski 2012). However, as noted above, bin schemes are also uncertain, and the spread of model solutions using different bin schemes can be quite large (vanZanten et al. 2011; Xue et al. 2017). Thus, it is imperative to devise strategies for improving how radar and satellite observations and other cloud and precipitation measurements can be used directly to constrain bulk microphysics schemes, which remain the mainstay of all operational models and most research models.

When new observational information is incorporated within a model, which is especially relevant for parameterizing microphysics, this can be posed as a Bayesian problem. When defined in this way, Bayes’s theorem defines the solution. In most problems, generally there is some vector \( x \) of quantities that we are interested in estimating (parameters), and some vector of observations \( y \), which usually do not (but may) include the parameters. The forward model \( f(x) \) takes in values of the control parameters and returns simulated output. We are usually interested in the “posterior probability” \( P(x|y, f) \), which can be read as “the probability of values of parameters \( x \) given the observations \( y \) and the model \( f(x) \).” Bayes’s theorem solved for this posterior probability is written

\[
P(x|y, f) = \frac{P(y|x, f)P(x|f)}{P(y|f)},
\]

where \( P(y|x, f) \) is the “likelihood,” a measure of the mismatch between the observations and forward simulations, \( P(x|f) \) is prior information or conjecture on the parameter values, and \( P(y|f) \) is a normalizing constant, sometimes called “evidence” and typically ignored for parameter estimation or uncertainty quantification problems.

Bayes’s theorem is especially relevant for microphysics because empirical advances by necessity play a critical role in scheme development. Nonetheless, the setting or tuning of uncertain parameter values and testing of the effects of parameter perturbations typically has been rather ad hoc. A few recent studies have used Bayesian techniques to rigorously constrain parameter distributions in bulk microphysics schemes using synthetic “observations” (e.g., Posselt and Vukicevic 2010; van Lier-Walqui et al. 2012, 2014; Posselt 2016). These studies solved (1) to characterize the model response to parameter changes (i.e., uncertainty quantification), as well as to optimize parameter settings for a given set of observational information. None of these studies used real observations; as such, they only explored the theoretical constraint of model-generated synthetic observations with prescribed uncertainty for a limited set of parameters in an idealized framework. Relatedly, Johnson et al. (2015) used a Gaussian process emulator to quantify the propagation of microphysical parameter uncertainty in a cloud model. An assumption implicit in these kinds of studies is that model uncertainty is fully captured by the set of parameters that are perturbed. For microphysics, this is questionable because there are a large number of parameters in current state-of-the-art bulk schemes (generally 25 or more), whereas typically only a subset of them are varied (up to \( \sim 10 \)). Even if uncertainty in all traditional parameters could be taken into account (e.g., those controlling particle densities, collection efficiencies, and terminal fall speeds), there are also several sources of structural uncertainty within schemes. These include 1) uncertainty in the functional forms for process rates, or from processes that are neglected entirely; 2) uncertainty in the functional forms of the particle size distributions; and 3) uncertainty associated with the numerical methods solving the model microphysical and dynamical equations. It can be very difficult to isolate these structural and parametric sources of uncertainty given the design of current microphysics
schemes, with implications for parameter estimation, assimilation of observations, propagation of uncertainty in models, and ensemble prediction. These different sources of uncertainty motivated van Lier-Walqui et al. (2014) to perturb microphysical processes directly within a Bayesian framework, as opposed to parameters. The problem of isolating various sources of uncertainty may be exacerbated by the development of increasingly complex microphysics schemes, with the added complexity and increased degrees of freedom necessitating additional parameters that are often poorly constrained by theory or observations. Moreover, greater complexity means larger parameter space dimensionality, making it more difficult to use Bayesian methods to quantify uncertainty and constrain parameters using observations. Thus, we argue that the increasing complexity of schemes may be moving ahead of our fundamental ability to constrain them systematically using observations, resulting in uncertainty that is increasingly difficult to understand and quantify.

An alternative approach is to combine the current fundamental but inherently limited knowledge of microphysical processes with an ability to robustly constrain uncertainty using the wealth of observational data (e.g., polarimetric radar) now available—in effect, applying Bayes’s theorem to optimally assimilate observations and estimate uncertainty. Not only would this make better use of observations for constraining schemes compared to current methods, but the ability to quantify uncertainty more systematically and robustly would indicate where to focus efforts to improve process-level knowledge of microphysics, and could provide insights for improving the representation of uncertainty for ensemble weather and climate prediction. This approach is in the spirit of Schneider et al. (2017), who advocated using machine learning and assimilation methods to constrain parameters while keeping an explicit connection to the underlying physics. Broadly, the idea here is to incorporate existing process-level knowledge and strictly enforce integral constraints, while using Bayesian inference to determine uncertain microphysical process representations.

Another approach is to develop full parameterizations using machine learning without specifying any explicit underlying physical framework (e.g., Rasp et al. 2018; Gentine et al. 2018; O’Gorman and Dwyer 2018; Brenowitz and Bretherton 2018). For example, this was recently applied using deep neural network learning to parameterize all subgrid-scale processes in a global climate model using training data from a high-resolution cloud model (Rasp et al. 2018). Although Rasp et al. (2018) demonstrated the success of this approach, particularly given that physical constraints (in their case, energy conservation) were well approximated through learning, here we retain a connection to specific microphysical processes. We argue that with only limited theoretical guidance available and no benchmark microphysics model, the physical constraints that do exist are particularly valuable to incorporate into microphysics schemes. Utilizing a physical framework also improves interpretability and physical meaning of the approach. Further, we believe that uncertainty quantification, which is facilitated using Bayesian inference, is an essential component of observationally constraining microphysics schemes. This is because observations alone are unlikely to provide sufficient information content to uniquely or unambiguously determine process rates.

Based on these ideas, a new statistical–physical framework is proposed for parameterizing microphysics—the Bayesian Observationally Constrained Statistical–Physical Scheme (BOSS). Recognizing that both structural and parametric sources of uncertainty are a fundamental and unavoidable aspect of microphysics, this approach incorporates elements from statistical modeling and Bayesian inference together with existing, though limited, process-level microphysical understanding. The number of parameters is limited to the extent possible in order to minimize the parameter dimensionality and complexity, making Bayesian methods more tractable. In other words, scheme complexity is designed to be at a level commensurate with our ability to constrain it observationally using Bayesian techniques. Parameters in the scheme have a well-defined physical meaning, so that uncertainty in a parameter can be traced to a specific physical process or feature. Other desirable features of traditional schemes are retained, including strict enforcement of water and energy conservation and positive definiteness of cloud and precipitation quantities. Finally, the framework is designed so that complexity can be added systematically. Increasing the number of terms in the process rate formulations and/or increasing the number of prognostic microphysical variables, both of which increase the number of parameters, allows systematic testing and quantification of structural uncertainty. The level of complexity can be tailored to any set of available observations, and increased as appropriate when new observations or theoretical advances become available. By design, the process rate formulations in their most general form span the set of all arbitrary smooth functions. Thus, the scheme can account for a huge degree of structural uncertainty while retaining the framework of using parametric, physically based equations to evolve the model prognostic state variables. This statistical–physical approach is therefore flexible and general.

The approach is described in the current paper (Part I), along with idealized tests illustrating its behavior.
van Lier-Walqui et al. (2020, hereafter Part II) describe application in idealized experiments for parameter estimation, uncertainty quantification, and forward propagation of model uncertainty using Markov chain Monte Carlo (MCMC) sampling to solve Bayes’s equation [see (1)]. The purpose of these papers is to document the new framework and show “proof of concept.” For simplicity, we restrict the initial development to rain microphysics, as it is relatively simple and rain observations are widely available from ground-based and spaceborne radar. Moreover, rain processes are critical for many systems including precipitating convection through their influence on cold pools and convective dynamics (e.g., Gilmore and Wicker 1998; Morrison et al. 2012; Li et al. 2015; Lombardo and Kading 2018).

The rest of the paper is organized as follows. Section 2 gives an overview of BOSS. Section 3 describes idealized one-dimensional tests to illustrate its behavior. Discussion and conclusions are provided in section 4.

2. Description of the approach

In designing a scheme (BOSS) that incorporates the basic features outlined in the introduction, we are necessarily constrained by the basic physics of the problem. Although there may be debate regarding what is considered accepted knowledge, there is a well-agreed-upon set of basic features of rain microphysics: drops sediment and grow by collision–coalescence, collisional breakup increases drop number, and drops falling into subsaturated conditions evaporate as a function of relative humidity, modified by ventilation effects. In supersaturated conditions, drops grow by vapor diffusion.

We have designed a simple yet flexible set of equations that captures these fundamental processes. A schematic diagram of BOSS is shown in Fig. 1. Fundamental though limited process-level knowledge informs the process rate formulations described below. These general formulations have an adjustable number of terms and parameter values and compose the microphysical model. The model is run through a Bayesian algorithm (MCMC in Part II), which uses observations of bulk rain properties (e.g., radar polarimetric variables) to constrain the number of process rate terms and parameter values. The outputs are a set of observationally constrained process rate parameterizations.

Prognostic microphysical variables in BOSS are the DSD moments, where the $k$th-order moment is a weighted integral of the DSD defined by

**The Bayesian Observationally-constrained Statistical-physical Scheme (BOSS)**

![Diagram of BOSS](http://journals.ametsoc.org/doi/pdf/10.1175/JAS-D-19-0070.1)

Fig. 1. Schematic diagram of BOSS. Prior microphysical knowledge in box 1 informs the process rate formulations in box 2. This knowledge includes the number of processes and their type (single-drop or drop–drop interaction), and the coupling of processes with the thermodynamic state variables through $F(T, p, q)$. It may also include information on the prior parameter distributions (e.g., parameter ranges). The process rate formulations in box 2 are general and flexible with an adjustable number of terms and parameter values. The process rate formulations comprise the model that is trained using a Bayesian machine learning approach that incorporates observations of bulk rain properties (e.g., radar polarimetric variables) in box 3. The output is a set of observationally constrained process rate parameterizations.
and $N' = \partial N/\partial D$ is the DSD function, expressed by the total number mixing ratio of drops (number of drops per kg of dry air) between diameters $D$ and $D + dD$. Physically, the DSD moments correspond to extensive quantities such as bulk number mixing ratio ($M_0$) and bulk mass mixing ratio times $6/(\pi \rho_v) (M_3)$ where $\rho_v$ is the density of liquid water.

The conservation equation for any prognostic moment $M_k$ is

$$
\frac{\partial M_k}{\partial t} + \mathbf{u} \cdot \nabla M_k + \rho_a^{-1} \frac{\partial (\rho_a V_k M_k)}{\partial z} = \left( \frac{dM_k}{dt} \right)_{\text{diff}} + \left( \frac{dM_k}{dt} \right)_{\text{coal}} + \left( \frac{dM_k}{dt} \right)_{\text{break}} + \Psi(M_k),
$$

where $t$ is time, $\mathbf{u}$ is the wind vector, $\rho_a$ is air density, $V_k$ is the mean fall speed weighted by $M_k$, and $\Psi$ is a diffusion/subgrid-scale mixing operator. The time derivatives on the right-hand side are the rain microphysical process rates: evaporation/condensation (diff), collision–coalescence (coal), and collisional breakup (break). Spontaneous breakup is neglected as process studies have shown it to be unimportant for rain (Pruppacher and Klett 1997). Formulations for each of these processes are described below.

### a. Process rate formulations

Rain processes are grouped into two categories. The first includes processes that act on individual drops, namely, evaporation/condensation and sedimentation. The second includes processes that involve drop–drop interactions, namely, collision–coalescence and collisional breakup. Following (3), BOSS requires equations for the time change of prognostic DSD moments. Taking $d/dt$ of (2) gives the time rate of change of moment $M_k$ from a microphysical process:

$$
\frac{dM_k}{dt} = \int_{D_{\min}}^{D_{\max}} (N' dD) k D^{k-1} + D^k \frac{\partial N'}{\partial t} \ dD.
$$

The first term in the integral is the growth or shrinkage of existing drops, and the second term accounts for the loss of existing drops or generation of new drops.

1) SINGLE-DROP PROCESSES

For processes acting on individual drops, $dD/dt$ can only be a function of some measure of the drop, that is, $D$, as well as the thermodynamic state variables (temperature $T$, pressure $p$, water vapor mixing ratio $q$, and other chemical constituents that are hereafter neglected). Thus, we write $k D^{k-1} dD/dt = g_k(D, T, p, q)$. The term $D^k \partial N'/\partial t$ in (4) from a process acting on individual drops (the loss of drops from evaporation) can also only depend on some measure of the drop and the thermodynamic state variables, and must scale with the number of drops from $D$ to $D + dD$, that is, $N'$. Thus, we express $D^k \partial N'/\partial t = h_k(D, T, p, q) N'$. Combining these expressions with (4) gives

$$
\frac{dM_k}{dt} = F(T, p, q) \int_{D_{\min}}^{D_{\max}} f_k(D) N' \ dD,
$$

where it is assumed that the functional dependencies on the state thermodynamic variables and $D$ can be written as separable functions: $g_k(D, T, p, q) + h_k(D, T, p, q) = F(T, p, q) f_k(D)$. Note this assumption potentially introduces some structural uncertainty, but this is not expected to be a large source of error. Current bulk schemes generally neglect any nonseparable dependencies on thermodynamic state variables and $D$ for process rates, with the exception of ventilation effects on drop evaporation [see (A7) in the appendix]. However, tests assuming constant thermodynamic parameters for ventilation, so that these parameters can be pulled into $F(T, p, q)$ outside of the integral in (5), show impacts on bulk evaporation rates of a few percent or less (see the appendix for details). The exact form of $f_k(D)$ is assumed to be unknown, but expressible as a generalized power series (e.g., Loeb 1991) of $D$:

$$
f_k(D) = \sum_{j=1}^{J} a_{j,k} D^{j b_k},
$$

where $a'$ and $b'$ are coefficients, $j$ is a counting index for terms in the sum, and $J$ is the total number of terms.

Process rates are formulated using generalized power expressions because these expressions encompass the set of all arbitrary smooth functions. Thus, process rates that follow any arbitrary smooth function can in principle be described within this framework. Generalized power expressions also allow for systematic probing of structural uncertainty by increasing the number of terms as the “true” process rate is approached, assuming it follows a smooth functional relationship. Furthermore, this approach provides continuity with the process rate formulations in traditional bulk schemes, which often conform to generalized power expressions using one or two terms as shown in the appendix.

If a function is continuous over a closed interval, it can be approximated as closely as desired over that interval.
by a polynomial according to the Weierstrass approximation theorem, and thus by generalized power series as well because they encompass the set of all polynomials. As discussed in Morrison et al. (2019), although polynomial approximation is straightforward and efficient, several terms may be needed for accuracy to fit even simple functions such as single-term power functions with noninteger exponents. Because generalized power series encompass the set of all polynomials, equal or greater accuracy using power series fits is obtained for the same number of terms. However, fitting can be more challenging when using more than one term in generalized power expressions. This issue is detailed in Part II in the context of MCMC sampling.

Combining (5) and (6) and expressing the integrals as moments gives

\[
\frac{dM_k}{dt} \approx F(T, p, q) \sum_{j=1}^{J} \delta_{j,k} M_{j/k}^{\beta_{j,k}},
\]

(7)

To close the equations, we must relate \( M_{j,k} \) to the set of prognostic moments. Thus, on a fundamental level, bulk microphysics parameterization is a closure problem, conceptually similar to the turbulence closure problem as pointed out by Kogan and Belochitski (2012). Closure could be achieved by assuming a functional form for \( N \) (e.g., assuming a gamma DSD), which is the approach taken by traditional bulk microphysics schemes. Then parameters for bulk process rates for various prognostic moments can be related to one another analytically. However, to retain generality we do not assume a DSD form here, and instead relate moments to one another statistically.

The most general approach is to express each \( M_{j,k} \) as a multivariate generalized power series of the set of prognostic moments:

\[
M_{j,k} \approx \sum_{i=1}^{I} \alpha_{i,j,k} \prod_{n=1}^{N} \left( \frac{M_{p_n}}{M_{p_1}} \right)^{\beta_{i,j,k}},
\]

(8)

where \( M_{p_1}, M_{p_2}, \ldots, M_{p_N} \) are the \( N \) prognostic DSD moments, \( n \) is a counting index for the prognostic moments, \( i \) is a counting index for terms in the sum, \( I \) is the total number of terms, and \( \alpha' \) and \( \beta' \) are coefficients. When combined with (6) using a single term, this gives the same bulk process rate expressions as Kogan and Belochitski (2012). However, we can instead use the existence of intrinsic scaling relationships among DSD moments derived from DSD normalization. Following the normalization procedure proposed by Morrison et al. (2019), we relate \( M_{j,k} \) to two or more prognostic moments using

\[
M_{j,k} \approx M \sum_{i=1}^{I} \alpha_{i,j,k} \prod_{n=1}^{N-1} \left( \frac{M_{p_n}}{M_{p_1}} \right)^{\beta_{i,j,k}},
\]

(9)

Combining (9) and (7) and rearranging terms gives

\[
\frac{dM_k}{dt} \approx F(T, p, q) \sum_{j=1}^{J} \delta_{j,k} M_{j,k}^{\beta_{j,k}},
\]

(10)

where \( k \in \{p_1, p_2, \ldots, p_N\} \). This expression can be written as a single sum:

\[
\frac{dM_k}{dt} \approx F(T, p, q) \sum_{l=1}^{L} \alpha_{l,k} M_{l}^{\beta_{l,k}},
\]

(11)

for two-moment BOSS, where we have dropped subscript \( n \) for convenience, and

\[
\frac{dM_k}{dt} \approx F(T, p, q) \sum_{l=1}^{L} \alpha_{l,k} M_{l}^{\beta_{l,k}},
\]

(12)

for three-moment BOSS. In both (12) and (13) we have dropped subscript \( l \) for convenience.

2) DROP–DROP INTERACTION PROCESSES

Drop–drop interaction processes are fundamentally different from single-drop processes because they no longer depend on a single measure of drop size, but on the measures of the two interacting drops, that is, diameters \( D \) and \( D^* \) (here we assume that the outcome of any interaction between a drop pair is unaffected by simultaneous interaction with other drops). For drop–drop interaction processes, the growth of existing drops by collision–coalescence, \( kD^{k-1}dD/dt \), depends on the interaction of drops
having diameter $D$ with all other drops across the DSD having diameter $D^*$, as well as the thermodynamic state variables. Thus, we can write $kD^{k-1}dD/dt = \int_{D_{min}}^{D_{max}} g_{k}(D, D^*, T, p, q) (\partial N/\partial D^*) dD^*$. Similarly, the generation or depletion of drops from collection and breakup, $D^{k} \partial N/\partial d$, depends on the interactions of drops having diameter $D$ with all other drops having diameter $D^*$ and the thermodynamic state variables, and must scale with the number of drops between $D$ and $D + dD$, that is, with $N$. Thus, we can write $D^{k} \partial N/\partial d = N' \int_{D_{min}}^{D_{max}} h_{k}(D, D^*, T, p, q) (\partial N/\partial D^*) dD^*$. Combined with (4) and using the definition $N' = \partial N/\partial D$, these expressions give

$$
\frac{dM_k}{dt} \approx F^*(T, p, q) \int_{D_{min}}^{D_{max}} f_k(D, D^*) \frac{\partial N}{\partial D^*} dD^* dD,
$$

(14)

where again it is assumed that the dependencies on the state thermodynamic variables and $(D, D^*)$ in $g_k$ and $h_k$ can be written as separable functions: $g_k(D, D^*, T, p, q) + h_k(D, D^*, T, p, q) = F^*(T, p, q) f_k(D, D^*)$. The exact form of $f_k$ assumed to be unknown, but expressible as a generalized bivariate power series of $D$ and $D^*$:

$$
f_k(D, D^*) \approx \sum_{i=1}^{l} a'_{i,k} D^{p_i} D^{q_i} c'_i k,
$$

(15)

where $a'$, $b'$, and $c'$ are coefficients. Combining (14) and (15) and expressing the integrals in terms of moments gives

$$
\frac{dM_k}{dt} \approx F^*(T, p, q) \sum_{i=1}^{l} a'_{i,k} M_{p_i, q_i}^{n-i} M_{q_i}^{n},
$$

(16)

We apply the normalization of Morrison et al. (2019) following a similar approach to the single-drop process rates. Combining the normalization in (9) with (16) gives

$$
\frac{dM_k}{dt} \approx F^*(T, p, q) a_k M_{p_1, p_2}^{n-i} M_{q_1, q_2}^{n},
$$

(17)

for two-moment BOSS, where we have dropped subscript $n$ for convenience, and

$$
\frac{dM_k}{dt} \approx F^*(T, p, q) a_k M_{p_1, p_2}^{n-i} M_{q_1, q_2}^{n},
$$

(18)

for three-moment BOSS. Subscript $l$ is dropped in both (20) and (21) for convenience.

Comparing (11)–(13) with (19)–(21), it is seen that process rates acting on individual drops have a somewhat different functional form than those associated with drop–drop interactions, namely, there is a dependence on $M_{p_1}^{\beta_{1,k}}$ for the former and $M_{p_2}^{\beta_{2,k}}$ for the latter (i.e., “1” vs “2” in the exponent). This is a direct consequence of the single-drop process rates being functions of $D$, whereas the multidrop process rates are functions of two diameters $D$ and $D^*$, combined with the DSD normalization. Using the generalized power expression in (8) to relate moments directly instead of the DSD normalization leads to the same functional form for both single-drop and multidrop process rates:

$$
\frac{dM_k}{dt} \approx F(T, p, q) \sum_{i=1}^{l} a'_{i,k} M_{p_i, q_i}^{n-i} M_{q_i}^{n},
$$

(19)

for two-moment BOSS, where we have dropped subscript $n$ for convenience, and

$$
\frac{dM_k}{dt} \approx F(T, p, q) a_k M_{p_1, p_2}^{n-i} M_{q_1, q_2}^{n},
$$

(20)

for three-moment BOSS. Subscript $l$ is dropped in both (20) and (21) for convenience.

Using single terms in each of the sums, (19) is simplified to

$$
\frac{dM_k}{dt} \approx F^*(T, p, q) a_k M_{p_1, p_2}^{n-i} M_{q_1, q_2}^{n},
$$

(21)

for three-moment BOSS. Subscript $l$ is dropped in both (20) and (21) for convenience.

Note that the impact of applying normalization to relate moments rather than the generalized power series is
reduced as the number of prognostic moments is increased. In other words, although the normalization is built in to the process rate functional forms, these forms approach the nonnormalized ones as the number of terms is increased. Thus, in principle they still encompass the set of all smooth functional forms for the process rates. However, using normalization does decrease the total number of parameters, which may be important for constraint of parameters using Bayesian estimation methods, which typically become less efficient for large parameter dimensionality.

The set of equations derived in this section is the forward model part of BOSS, which is the focus of this paper. The Bayesian inference component is detailed in Part II, and hence only briefly described here. Within BOSS, Bayesian inference is used to estimate posterior probability density functions (PDFs) of the process rate parameters within the scheme (the forward model), given prior PDFs of the parameters and a vector of observations with a defined observational uncertainty. This provides not only the maximum a posteriori (most probable) parameter values, but also the full probability distributions across the multidimensional parameter space. In Part II, we use MCMC as the Bayesian inference algorithm within BOSS using constraint by synthetic “observations.” In MCMC, posterior parameter PDFs are estimated using a sequence of forward model calculations that map out the probability space. For simplicity, the prior parameter PDFs are assumed uniform with bounds designed to encompass the high probability regions of the posterior parameter PDFs. Additional information, for example, from detailed microphysics schemes or theory, could be used to more stringently bound the prior parameter PDFs. In Part II, the posterior parameter PDFs are estimated using 20 to 40 cases with BOSS coupled to a steady-state rainshaft model; each case has varying upper boundary conditions for the rainshaft (i.e., different values for the prognostic moments specified at the model top). For these calculations, the structural form of the process rates is assumed a priori by setting the number of process rate terms (either 1 or 2 are used) and prognostic moments (2 or 3); this forms the basis for a simple investigation of structural uncertainty described in Part II. We also note the possibility of using Bayesian techniques for model selection (e.g., Sambridge et al. 2013) to estimate the posterior parameter PDFs within BOSS as well as the number of process rate terms and prognostic moments accounting for both fit accuracy and parsimony.

Although BOSS uses Bayesian inference for estimating parameters of the process rate power expressions, it retains a high degree of interpretability. This is because the parameters correspond to individual process rates that have a specific physical meaning. Moreover, the Bayesian framework of BOSS provides a rigorous way to incorporate existing theoretical or empirical knowledge about the process rates through the specified prior parameter distributions, or by modifying the number of process rate terms (see Part II for more discussion). This is important, and it means that any improvements in fundamental microphysical knowledge can be incorporated into BOSS systematically. Interpretability is also retained by noting an explicit connection between the generalized power expressions derived above and the process formulations in traditional bulk schemes. As shown in the appendix, some process formulations in a traditional bulk microphysics scheme (Morrison et al. 2009) exactly conform to the general BOSS process rate expressions using one or two terms, though others do not (collision–coalescence and collisional breakup).

An advantage of the BOSS framework compared to traditional schemes is that it is extremely flexible; any combination or number of prognostic moment variables can be used. Thus, prognostic variables for a two-moment approach do not have to be the traditional choice of $M_0$ and $M_3$. For example, the combination of $M_3$ and $M_6$ is tested in section 3, which may be desirable for some applications because $M_6$ is the radar reflectivity factor and is directly proportional to the observed equivalent radar reflectivity factor if particles are small compared to the wavelength of the radar signal. Further, the prognostic variables do not have to be integer moments, which may be useful for some applications when observed quantities are proportional to noninteger moments, such as rain flux. In addition to the benefits of consistency between the prognostic moments and bulk observations, the practical choice of prognostic variables is governed by 1) the level of complexity appropriate for a given set of observations, because the number of uncertain parameters to be constrained increases by adding prognostic variables; 2) computational efficiency, which decreases with the number of prognostic variables. Although not a requirement, in most applications it is desirable to prognose $M_3$ (because it is proportional to bulk mass) to ensure conservation of total water mass and also because bulk mass is needed for calculating buoyancy. Moreover, prognosing $M_3$ reduces the total number of parameters needed compared to prognosing other moments because collision–coalescence and collisional breakup do not change bulk mass.

### b. Evaporation/condensation

Vapor diffusion acts on individual drops, and the expression for $(dM_k/dt)_{\text{diff}}$ is thus given by (11). In the general case, all moments of the DSD are impacted by $(dM_k/dt)_{\text{diff}}$.  

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The thermodynamic function $F(T, p, q)$ neglecting ventila-
tion follows from Byers (1965), and is expressed as

$$F_{\text{diff}}(T, p, q) = \frac{12\rho_w D_q S_q}{\rho_w \left(1 + \frac{d\alpha}{dT}(1) c_p\right)}, \quad (23)$$

where $\rho_w$ is the density of liquid water, $D_q$ is the diffu-
sivity of water vapor, $S$ is the supersaturation ratio ($S =
q/a(q - 1)$), $q_v$ is the water vapor mixing ratio, $q_i$ is the
saturation mixing ratio, $L_w$ is the enthalpy of vaporization,
and $c_p$ is the specific heat of air at constant pressure. Note
that (23) is the thermodynamic term for the change in $M_3$
from evaporation/condensation, and thus is different from
the analogous term for the change in bulk mass by a factor
of $(\pi/6)\rho_w$. Modification to account for ventilation of drops
in BOSS is discussed in the appendix.

c. Collision–coalescence and collisional breakup

The expression for $(dM_k/dt)_{\text{coal}}$ is given by (19) with
$F_{\text{coal}} = 1$. Similarly, $(dM_k/dt)_{\text{break}}$ is given by (19) with
$F_{\text{break}} = 1$. For both, $(dM_3/dt)_{\text{coal}} = 0$ and $(dM_3/dt)_{\text{break}} = 0$
because bulk mass does not change from collision–
coalescence and collisional breakup. There is also a
constraint on the sign of the change in $M_k$ from
collision–coalescence and breakup depending on the
moment order $k$. Collision–coalescence produces a
relative shift in the DSD toward larger drops. Thus, the
ratio $(M_i/M_k)^{i-k}$ must increase for any moment orders
$i \geq 0$ and $k \geq 0$, where $i \neq k$. Because the change in $M_3$
is zero and $M_3/M_k$ must increase from collision–
coalescence for all $k \geq 0$ and $k \neq 3$, the change in $M_k$
from collision–coalescence must be <0 for $k < 3$. Similarly,
because the ratio $M_k/M_3$ also must increase for $k > 3$,
the change in $M_k$ from collision–coalescence must be >0 for $k > 3$. The opposite occurs for breakup,
with a relative shift of the DSD to smaller drop sizes.
The change in $M_k$ from breakup must therefore be >0
for $k < 3$, and <0 for $k > 3$.

Note that because they use the same process rate forms
and $F_{\text{coal}} = F_{\text{break}}$, formulating collision–coalescence
and collisional breakup each using (19) with $L$ terms is
mathematically equivalent to representing the combina-
tion of collision–coalescence–breakup using (19) with $2L$
terms, with half the terms being opposite in sign to the
other half following the integral constraint discussed
above. This illustrates how it is the thermodynamic
function $F$, process type (single-drop vs drop–drop
interaction), and integral constraints that distinguish
processes from one another in BOSS. This issue is
further discussed from the standpoint of observational
constraint, process rate parameter fitting, and poste-
rior parameter distributions in Part II.

d. Sedimentation

Sedimentation acts upon individual drops. Following
(3), the gravitational flux in the conservation equation
for any prognostic moment $M_{p_k}$ is $\rho V_{p_k} M_{p_k}$. Expressions
for the moment-weighted mean fall speed $V_{p_k}$ are ob-
tained from dividing the general single-drop process rate
formulation (11) by $M_{p_k}$. The thermodynamic function
$F_{\text{fall}} = (\rho/\rho_0)^{0.54}$ following Heymsfield et al. (2007),
where $\rho_0$ is the air density at the bottom level. Because
fall speed increases monotonically with drop size, we
apply a physical constraint on the $i$th and $j$th moment-
weighted mean fall speeds that requires $V_i < V_j$ for
any moment orders $i < j$. We also apply the physical constraint
that $V_{p_k} < 10 \text{ m s}^{-1}$ for any $p_k \geq 0$, to conform with the fall
speeds of the liquid drops that occur in the atmosphere.

For the two-moment BOSS using a single term in the
sum, this gives

$$V_{p_1} = F_{\text{fall}} d_{p_1} M_{p_1}^{1 - \beta_{p_1}} M_{p_1}^\beta_{p_1} = F_{\text{fall}} d_{p_1} M_{p_1}^{1 - \beta_{p_1}} M_{p_1}^\beta_{p_1}, \quad (24)$$

$$V_{p_2} = F_{\text{fall}} d_{p_2} M_{p_2}^{1 - \beta_{p_2}} M_{p_2}^\beta_{p_2} = F_{\text{fall}} d_{p_2} M_{p_2}^{1 - \beta_{p_2}} M_{p_2}^\beta_{p_2}, \quad (25)$$

where $\hat{\beta}_{p_2} = \beta_{p_1} - 1$.

For the three-moment BOSS using a single term, this
gives

$$V_{p_1} = F_{\text{fall}} d_{p_1} M_{p_1}^{1 - \beta_{p_1}} M_{p_2}^{\beta_{p_1} - \beta_{p_2}} M_{p_3}^{\beta_{p_1}} = F_{\text{fall}} d_{p_1} M_{p_1}^{1 - \beta_{p_1}} M_{p_2}^{\beta_{p_1} - \beta_{p_2}} M_{p_3}^{\beta_{p_1}}, \quad (26)$$

$$V_{p_2} = F_{\text{fall}} d_{p_2} M_{p_2}^{1 - \beta_{p_2}} M_{p_3}^{\beta_{p_2} - \beta_{p_3}} M_{p_3}^{\beta_{p_2}} = F_{\text{fall}} d_{p_2} M_{p_2}^{1 - \beta_{p_2}} M_{p_3}^{\beta_{p_2} - \beta_{p_3}} M_{p_3}^{\beta_{p_2}}, \quad (27)$$

$$V_{p_3} = F_{\text{fall}} d_{p_3} M_{p_3}^{1 - \beta_{p_3}} M_{p_2}^{\beta_{p_3} - \beta_{p_2}} M_{p_3}^{\beta_{p_3}} = F_{\text{fall}} d_{p_3} M_{p_3}^{1 - \beta_{p_3}} M_{p_2}^{\beta_{p_3} - \beta_{p_2}} M_{p_3}^{\beta_{p_3}}, \quad (28)$$

where $\hat{\beta}_{1,p_1} = \beta_{1,p_1} - 1$, $\hat{\beta}_{1,p_3} = \beta_{1,p_3} - 1$, and $\hat{\beta}_{2,p_3} = \beta_{2,p_3} - 1$.

3. Idealized one-dimensional rainshaft tests

a. Description

Idealized one-dimensional (1D) tests are presented to
illustrate behavior of BOSS. We compare solutions using
different configuration of BOSS with those from a traditional bulk microphysics scheme across a wide range of conditions. The point is not to recreate solutions from the traditional scheme, but to demonstrate that similar solutions exist within the parameter space of BOSS, which utilizes a set of power-law equations to represent the process rates as detailed in section 2.

Because rain processes are the focus of this work, tests were performed with a 1D model representing a steady-state rain shaft. Air motion is assumed to be zero. Because steady state is explicitly assumed, \( \frac{\partial}{\partial t} = 0 \) and the conservation equation for any prognostic moment is

\[
\rho_a \frac{\partial (\rho_a V_k M_k)}{\partial z} = (\frac{dM_k}{dt})_{\text{diff}} + (\frac{dM_k}{dt})_{\text{coal}} + (\frac{dM_k}{dt})_{\text{break}}.
\]

Integration over height \( z \) is done using a simple forward Euler method. The number of vertical levels is 80, with a grid spacing of 25 m and a 2-km-deep domain. Specified values of \( M_0 \) and \( M_3 \) at the model top (\( M_{0,\text{top}} \) and \( M_{3,\text{top}} \)) are an upper boundary condition for the two-moment schemes, with \( M_6 \) also specified at the top (\( M_{6,\text{top}} \)) for the three-moment schemes. In these tests, profiles of temperature and \( q_a \) are held fixed at the dry adiabatic lapse rate and a constant relative humidity (RH). The surface temperature is 297.15 K. The profile of air pressure is hydrostatic with a surface pressure of 10^5 Pa. A large number of tests were performed with various RH (0.2 to 1), \( M_{3,\text{top}} \) (0.91 \times 10^{-9} \text{ to } 7.64 \times 10^{-6} \text{ m}^3 \text{ m}^{-3} \), corresponding to mass concentrations of \( 1 \times 10^{-6} \text{ to } 4 \times 10^{-3} \text{ kg m}^{-3} \), and \( M_{0,\text{top}} \) (1.05 \times 10^6 \text{ to } 1.05 \times 10^{10} \text{ times } M_2 \text{ units of } M_0 \text{ are } m^{-3} \). For the three-moment schemes, \( M_{6,\text{top}} \) corresponds to either inverse exponential DSDs (gamma with \( \mu = 0 \)) or those of a gamma DSD with \( \mu = 10 \), where the gamma DSD is expressed as

\[
\frac{\partial N}{\partial D} = N_0 D^\mu e^{-\lambda D}.
\]

Here \( \mu, N_0, \) and \( \lambda \) are the shape, intercept, and slope DSD parameters.

Table 1 describes the various BOSS and MORR configurations tested herein. Parameter settings for BOSS are detailed in the appendix. The two-moment BOSS configurations, M0-M3-B and M3-M6-B, are compared with the standard two-moment scheme of Morrison et al. (2009) (MORR-2MOM) that has \( M_0 \) and \( M_3 \) as prognostic rain variables. The three-moment configuration of BOSS, M0-M3-M6-B, is compared to a three-moment version of Morrison et al. (2009) with prognostic rain \( M_0, M_3, \) and \( M_6 \) (MORR-3MOM). MORR-2MOM produces similar responses to changes in \( M_{0,\text{top}}, M_{3,\text{top}}, \) and RH, although M0-M3-B produces larger rain rates (up to 70%) in the lowest-RH environments (Fig. 2a). This occurs because of larger evaporation owing to the inclusion of ventilation effects in MORR, as seen by vertical profiles of the \( M_0 \) and \( M_3 \) evaporation rates (Figs. 3, 4). M0-M3-B and MORR-2MOM produce similar responses to changes in \( M_{0,\text{top}}, M_{3,\text{top}}, \) and RH, although M0-M3-B produces larger rain rates (up to 70%) in the lowest-RH environments (Fig. 2a). This occurs because of larger evaporation owing to the inclusion of ventilation effects in MORR, as seen by vertical profiles of the \( M_0 \) and \( M_3 \) evaporation rates (Figs. 3, 4). M0-M3-B and MORR-2MOM produce similar responses to changes in \( M_{0,\text{top}}, M_{3,\text{top}}, \) and RH, although M0-M3-B produces larger rain rates (up to 70%) in the lowest-RH environments (Fig. 2a). This occurs because of larger evaporation owing to the inclusion of ventilation effects in MORR, as seen by vertical profiles of the \( M_0 \) and \( M_3 \) evaporation rates (Figs. 3, 4). M0-M3-B and MORR-2MOM produce similar responses to changes in \( M_{0,\text{top}}, M_{3,\text{top}}, \) and RH, although M0-M3-B produces larger rain rates (up to 70%) in the lowest-RH environments (Fig. 2a).
The two-term MORR formulation for evaporation that includes ventilation can be well approximated by using only a single term in BOSS but increasing the "a" parameter. Increasing this parameter by a factor of 5 gives rain rates that match very closely with MORR-2MOM (Fig. 5a) and fairly closely with MORR-3MOM (Figs. 5c,d), and thus can account reasonably well for the increased evaporation rate from ventilation in the more detailed MORR formulations. Vertical profiles of the prognostic moments, mean fall speeds, and process rates including evaporation are also similar to MORR using the enhanced "a" parameter in BOSS, for both the small and large mean drop size cases (Figs. 6, 7). We also show results for BOSS with prognostic $M_0$ and $M_3$ but using two terms for evaporation (M0-M3-B2), consistent with the formulation in MORR (see the appendix). Results are very similar to MORR-2MOM in terms of surface rain rates (Fig. 5b) and profiles for both the small (Fig. 6) and large (Fig. 7) mean drop size cases. Small differences between M0-M3-B2 and MORR-2MOM are mainly caused by somewhat different representations of collision–coalescence and breakup (see the appendix).

Vertical profiles are consistent with expectations of physical behavior. The weighted mean fall speeds show that $V_6 > V_3 > V_0$ (Figs. 3d–f and 4d–f), corresponding to the increase of fall speed with drop size. Large differences occur between the two-moment and three-moment representations of mean fall speed for both BOSS and MORR. M0-M3-M6-B and MORR-3MOM give only small differences between $V_0$, $V_3$, and $V_6$, whereas $V_3$ is about 3 times larger than $V_0$ in M0-M3-B and MORR-2MOM. These differences between the two- and three-moment schemes occur because the gamma DSDs specified at the model top are narrow for the cases in Figs. 3 and 4, with $\mu = 10$, which is inconsistent with the inverse exponential DSDs assumed in MORR-2MOM and corresponding to the parameter settings for M0-M3-B.

The small-drop case shows that collision–coalescence dominates breakup (Fig. 3g), leading to an increase of mean drop size from the model top toward the surface as
values approach the equilibrium mean size (not shown). In contrast, breakup dominates over coalescence for the large-drop case (Fig. 4g) so that mean drop size decreases rapidly toward the surface. This behavior is similar to MORR, which represents collision–coalescence together with collisional breakup as a single process, and is also consistent with rainshaft simulations using a detailed bin model as well as polarimetric radar observations (Kumjian and Prat 2014).

4. Discussion and conclusions

In this paper, BOSS was proposed for parameterizing rain microphysics. This approach was designed to facilitate constraint by observations and estimation of structural and parametric uncertainty using Bayesian inference. The basic idea was to combine fundamental knowledge of physical processes, which for microphysics is inherently limited, and Bayesian statistics within a physically based framework. Microphysical process rates were characterized by generalized power series of drop diameter $D$ for single-drop processes, and bivariate generalized power series of the two interacting drop diameters $D$ and $D^*$ for multidrop processes. Combined with the DSD normalization method from Morrison et al. (2019), we derived generalized power series expressions for the bulk process rates and moment-weighted mean
drop fall speeds that determine time tendencies of the prognostic DSD moment variables. The scheme is flexible and can utilize any number and combination of prognostic moments and any number of power terms for the process rate and mean fall speed expressions. Thus, complexity can be added and tested systematically.

This approach is somewhat related to the idea of using machine learning to guide parameterization development, which has been recently advocated (e.g., Schneider et al. 2017) and applied in weather and climate models (e.g., Rasp et al. 2018; Gentine et al. 2018; O’Gorman and Dwyer 2018; Brenowitz and Bretherton 2018). We point out the challenge of applying machine learning in a direct way to parameterize microphysics, given there is no benchmark microphysical model available to provide a comprehensive dataset for training to the “truth” (and indeed, without even the possibility of developing a true benchmark model given the lack of benchmark microphysical equations). Thus, we must rely heavily on indirect observations to inform microphysics schemes, combined with limited process-level microphysical knowledge, which is amenable to Bayesian methods. The relative lack of theoretical guidance for microphysics and reliance on observations for constraint arguably means the limited process-level knowledge that is currently available is particularly important to incorporate into parameterizations. Thus, we apply Bayesian inference within an explicit physical framework using a set of parametric equations, in the spirit of Schneider et al. (2017). The physical framework underlying BOSS also allows it to retain a degree of interpretability comparable to traditional bulk schemes, in contrast to “black box” approaches to data-driven parameterization development.

BOSS contrasts with existing bulk microphysics schemes in several ways. First, all process rate and moment relationships are expressed in terms of generalized power
expressions, contrasting with the explicit DSD and process rate functional forms assumed by most bulk schemes. Second, complexity can be added systematically by increasing the number of terms (and hence parameters) in the process rate power expressions, and/or by increasing the number of prognostic moments. Third, uncertainty resides within a limited, well-defined set of parameters. Thus, the framework is simpler and more flexible than existing approaches, facilitating direct constraint by observations. BOSS also allows systematic testing of both parametric and structural uncertainty, the latter by increasing the number of terms in the process rate formulations and/or increasing the number of prognostic moments.

We showed that some processes in a traditional bulk scheme (MORR) could be expressed analytically using the general forms in BOSS with one or two terms in the BOSS power expressions, but not others (collision–coalescence and collisional breakup). Nonetheless, BOSS produced similar results to two- and three-moment versions of MORR over a wide range of conditions for idealized 1D rainshaft tests. Thus, it can capture the nonlinear behavior of a traditional bulk microphysics scheme despite being simple and significantly different in philosophy and design. This point is further demonstrated in Part II using synthetic observations generated from the three-moment MORR scheme to rigorously constrain BOSS using MCMC. Ultimately, we envision the potential for BOSS to be used in weather and climate models by replacing the traditional bulk schemes in them in part or in whole, though several additional steps would need to be taken before this could be done. First, BOSS parameters would need to be estimated within the Bayesian framework, and there are some important considerations for this. For instance, it is unclear which real observations would be needed to constrain BOSS in practice, and this will likely depend on the particular model or application. For weather models, parameter estimation in the face of model state uncertainty, rapid error growth, and strong coupling between microphysical, dynamical, and thermodynamic
model variables is not straightforward. There are not yet general, widely used systems for simultaneous state and parameter estimation, although methods have been proposed (e.g., Laine et al. 2012). Climate modeling does not face the same problem of initial condition uncertainty and rapid growth of model state error, but there are other practical challenges for parameter estimation given the need to run forward model calculations within the Bayesian estimation framework for long enough to characterize model error statistically. Emulation-based approaches (e.g., Carslaw et al. 2013) might serve to mitigate this problem. Second, as a “proof of concept” we have initially focused on rain microphysics, but of course this is only a small part of the wider cloud-precipitation microphysical system. Substantial effort would be needed to extend the BOSS framework to all microphysical processes, and we are currently working to include cloud and warm rain initiation processes.

There are several potential advantages to formulating microphysics using the BOSS framework. The process rates are smooth and completely differentiable, facilitating the development of adjoints for variational data assimilation. The ability to address both parametric and structural sources of uncertainty systematically may help in the design of ensembles for weather and climate prediction. The quantification of uncertainty is built in to the framework directly, making studies of the propagation of this uncertainty straightforward using ensembles. This could be done, for example, by forward model calculations using parameter values sampled from the Bayesian observationally constrained posterior joint parameter distributions. Such sampling could be

Fig. 6. As in Fig. 3, but for M0-M3-BE, M0-M3-M6-BE, and M0-M3-B2, as indicated by the colored lines. M0-M3-BE and M0-M3-M6-BE are the BOSS configurations with the “a” parameter for evaporation enhanced by a factor of 5. M0-M3-B2 is the BOSS configuration with two-term evaporation.
done with parameter values fixed in time and space for each ensemble member, or parameter values could be stochastically varied in time and space.

Importantly, systematic characterization of structural uncertainty using BOSS can help elucidate the true uncertainty not captured by perturbing parameters in traditional schemes. This is because traditional schemes use fixed functional forms for process rates and DSDs and hence perturbing parameters in these schemes is unlikely to span the true uncertainty. Running multi-scheme ensembles (e.g., Hacker et al. 2011; Berner et al. 2015; Jankov et al. 2017) is a way to try and address structural uncertainty using traditional schemes, but this is not systematic and it is unclear how much of the true uncertainty is actually accounted for by this approach. Nonetheless, the relatively large spread of multiphysics ensembles using different schemes relative to parameter perturbation ensembles (Jankov et al. 2017) is indicative of the general importance of structural uncertainty. By design, the generalized power expressions for the process rate formulations in BOSS include the entire set of all smooth arbitrary functions (see section 2). Thus, they can span a very large range of structural uncertainty associated with the process rate formulations while still retaining a physical framework centered around a set of well-defined parametric equations. Nonetheless, there is still some structural uncertainty unaccounted for in the process rates from the thermodynamic terms $F(T, p, q)$, and the assumption that the thermodynamic variables $(T, p, q)$ are separate functions from the drop diameter(s). This could be accounted for in BOSS by writing the process rate formulations as multivariate generalized power expressions that include both the thermodynamic state variables and prognostic moments, but this was not explored here. There is also structural uncertainty from the numerical methods to solve the microphysical...
equations, an aspect also not explored here. Nonetheless, it should be pointed out that this structural uncertainty can be systematically tested in a straightforward way by standard numerical convergence tests.

The fact that BOSS is designed for ease of representation of microphysical parameterization uncertainty also means that it is well suited for other applications where quantifying microphysics knowledge is of interest. For example, BOSS can conceivably be used as a framework within which to retrieve microphysical process rates from columns of polarimetric radar observations. The probabilistic nature of BOSS allows for ascertaining whether polarimetric “fingerprints” of microphysical processes (e.g., Kumjian and Ryzhkov 2010; Kumjian and Prat 2014; Schrom et al. 2015; Kumjian and Lombardo 2017) can be unambiguously identified from observations. By contrast, existing methods typically make strong assumptions of DSD form (e.g., Williams 2016), or dominance by some singular process (e.g., Tridon et al. 2017).

In Part II, we investigate the constraint of BOSS with synthetic observations using MCMC with minimal a priori knowledge applied to the model. Thus, the prior parameter distributions are uniform with bounds that extend far enough to fully cover high density regions of the posterior parameter distribution space. The only explicit prior knowledge in the model comes from the process rate thermodynamic functions \( F(T, p, q) \) and the idea that certain processes act on individual drops or involve drop–drop interaction—in essence, what distinguishes processes from one another in the scheme (see section 2). Uncertainties associated with a priori assumptions are therefore a minimum. In essence, this allows us to ask a very basic question: In principle, what microphysical knowledge can be gained solely from a set of observations combined with only the most basic and certain a priori microphysical knowledge? Despite this rather severe limitation, as shown in Part II the process rates are well constrained. Because these experiments use synthetic observations, it is possible that, in practice, some additional a priori constraint may be needed to get meaningful results using real observations. This could be provided, for example, by knowledge from detailed models (bin or Lagrangian microphysics schemes) or laboratory studies to limit the bounds of the prior parameter distributions. We emphasize that BOSS is particularly well suited for this because of its flexibility, as it can systematically and rigorously combine observational constraint with any level of prior knowledge via Bayesian inference. The application of BOSS to real cases using polarimetric radar observations will be a focus of future work.

In the initial development of BOSS here and in Part II we focus on rain microphysics. This is because rain microphysics is relatively simple and well understood (compared to, e.g., ice microphysics), and there are extensive observations of rain and documented fingerprints of microphysical processes in rain from polarimetric radar (Kumjian and Prat 2014). Extensions of this framework to include other microphysical processes is an obvious future step. We have begun designing a version of BOSS that incorporates warm cloud processes, which requires additional prognostic moments in order to capture both cloud and rain processes simultaneously similar to the scheme of Kogan and Belochitski (2012). The inclusion of ice microphysics is also left to future work. This will present other challenges given the need to represent additional ice particle characteristics such as shape and density, which influence the evolution of ice-bearing cloud systems (e.g., Hashino and Tripoli 2007; Milbrandt and Morrison 2013; Jensen et al. 2018).

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APPENDIX

Parameter Settings for BOSS Tests

Here we detail parameter settings for the BOSS tests described in section 3. This also illustrates the connection between the traditional process formulations in MORR and the general formulations in BOSS, including analytic equivalency for some processes. All parameter settings are listed in Table A1 for M0-M3-B, Table A2 for M3-M6-B, and Table A3 for M0-M3-M6-B.

a. Sedimentation

We first show analytically how the moment-weighted mean fall speeds in MORR can be expressed exactly using the BOSS formulations with a single term in the sums. In MORR the mean fall speeds are derived by assuming a gamma DSD with \( \mu = 0 \) (inverse exponential) for rain. A power-law fall speed–\( D \) relationship is used following Liu and Orville (1969): \( V = a_s D^{b_v} \), where \( a_s = 841.99667 \text{m}^2 \text{s}^{-1} \) and \( b_v = 0.8 \). To derive the expressions below, we relate the gamma DSD parameters \( \lambda \) and \( N_0 \) to two prognostic moments \( M_{p_1} \) and \( M_{p_2} \), using the definition of a gamma DSD moment \( M_k = \int_0^\infty N_0 D^k e^{-\lambda D} dD = N_0 \Gamma(k + \mu + 1)\lambda^{-(k+\mu+1)} \).

\[
\lambda = \frac{M_{p_1}}{M_{p_2}} \frac{\Gamma(\mu + p_1 + 1)^{p_1}(p_1-p_2)}{\Gamma(\mu + p_1 + 1)} , \tag{A1}
\]
TABLE A1. Values of parameters for the M0-M3-B tests shown in section 3. Parameter values are derived analytically following MORR or chosen to produce results similar to MORR (see the appendix). Units of $a_k$ are $m^{-3}\cdot$h$^{-k-2}$ for evaporation, $m^{-3}\cdot$h$^{-k}$ s$^{-1}$ for collision–coalescence and breakup, and $m^{-1}\cdot$h$^{-k}$ s$^{-1}$ for the mean fall speeds. Here $k = 0$ for the $M_0$ rates and $V_G$; $k = 3$ for the $M_3$ rates and $V_5$.

<table>
<thead>
<tr>
<th>$a_k$</th>
<th>$\beta_k$, $\beta_k$, or $\delta_k$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$V_0$</td>
<td>$6^{-b/3}a_v \Gamma(1 + b_v)$ = 486.34 $b_v/3 = 0.26667$</td>
</tr>
<tr>
<td>$V_3$</td>
<td>$6^{-b/3}a_v \Gamma(4 + b_v)$ = 1552.38 $b_v/3 = 0.26667$</td>
</tr>
<tr>
<td>$(dM/dt)_{\text{evap}}$</td>
<td>$6^{-1/3} = 0.5503$ $-0.6667$</td>
</tr>
<tr>
<td>$(dM/dt)_{\text{coal}}$</td>
<td>$6^{-1/3} = 0.5503$ $0.3333$</td>
</tr>
<tr>
<td>$(dM/dt)_{\text{break}}$</td>
<td>$-4.5753 \times 10^{-2}$ $0.5$</td>
</tr>
<tr>
<td>$(dM/dt)_{\text{break}}$</td>
<td>$10.0 \times 10^3$ $2.3385$</td>
</tr>
</tbody>
</table>

$N_0 = \frac{M_{0,3}^{\lambda_{\mu} + p_{l/3 + 1}}}{\Gamma(\mu + p_{1/3} + 1)}.$ (A2)

For prognostic $M_0$ and $M_3$, analogous to the traditional prognostic number and mass mixing ratios in two-moment schemes, this gives for the $M_0$- and $M_3$-weighted mean fall speeds:

$$V_0 = \frac{\int_0^\infty F_{\text{fall}} a v N_0 D^{b/3} e^{-\lambda D} dD}{\int_0^\infty N_0 e^{-\lambda D} dD} = F_{\text{fall}} 6^{b/3} a_v \Gamma(1 + b_v) M_0^{b/3} M_3^{b/3/3},$$ (A3)

$$V_3 = \frac{\int_0^\infty F_{\text{fall}} a v N_0 D^{b+3} e^{-\lambda D} dD}{\int_0^\infty N_0 D^3 e^{-\lambda D} dD} = F_{\text{fall}} 6^{b/3} a_v \Gamma(4 + b_v) M_0^{b/3} M_3^{b/3/3}.$$ (A4)

These expressions are identical to (24) and (25), respectively, in BOSS with $a_{p1} = 6^{b/3} a_v$, $a_{p2} = 6^{-(b/3-1)} a_v \Gamma(4 + b_v)$, and $\beta_{p1} = \beta_{p2} = b_v/3$.

Similarly, for prognostic $M_3$ and $M_6$ we obtain

$$V_3 = \int_0^\infty F_{\text{fall}} a v N_0 D^{b/3} e^{-\lambda D} dD$$

$$= F_{\text{fall}} 6^{b/3} a_v \Gamma(4 + b_v) M_3^{b/3} M_6^{b/3/3},$$ (A5)

$$V_6 = \int_0^\infty F_{\text{fall}} a v N_0 D^{b/3} e^{-\lambda D} dD$$

$$= F_{\text{fall}} 6^{b/3} a_v \Gamma(7 + b_v) M_3^{b/3} M_6^{b/3/3},$$ (A6)

which are also identical to (24) and (25), respectively, in BOSS with $a_{p1} = [120^{b/3}]^6 a_v \Gamma(4 + b_v)$, $a_{p2} = [120^{b/3}]^6/20 a_v \Gamma(7 + b_v)$, and $\beta_{p1} = \beta_{p2} = b_v/3$.

The $M_0$, $M_3$, and $M_6$-weighted fall speeds for MORR-3MOM are also derived assuming gamma DSDs. This gives for $V_0$

$$V_0 = \int_0^\infty F_{\text{fall}} a v N_0 D^{b+3} e^{-\lambda D} dD$$

$$= F_{\text{fall}} a v \sigma_0 \left( \frac{M_0 M_3^{\lambda/2}}{M_3^{b/3}} \right) d_{\text{evap}} M_0^{b/3} M_3^{b/3/3}$$

$$= F_{\text{fall}} a v \sigma_0 M_0^{b/3 + d_{\text{evap}}} M_3^{b/3 - 2d_{\text{evap}}} M_{\text{evap}},$$ (A7)

which is identical to (26) in BOSS with $a_{p1} = a_v \sigma_0$, $\beta_{p1} = b_v/3 - d_{\text{evap}}$, and $\beta_{p2} = d_{\text{evap}}$, where $\sigma_0$ and $d_{\text{evap}}$ are fitted parameters as described below.

Because of the factor $X_{\text{evap}} = [\Gamma(1 + b_v + \mu)\Gamma(1 + \mu)][\Gamma(1 + \mu)\Gamma(4 + \mu)]^{b/3}$ in (A7), the mean fall speeds from MORR-3MOM do not conform exactly to the
First, we show how there is an exact correspondence with BOSS using a single term in the sum when ventilation effects are neglected, and with two terms in (A7). Values for the parameters $\sigma e_0$ and $d e_0$ are found by least squares fitting to $X_{d0}$ in log space across the relevant range of $(M_0 M_6/M_5^2)$ and given in Table A4.

Similarly, we obtain expressions for the $M_3$- and $M_6$-weighted mean fall speeds:

$$V_3 = \lim_{\rho \to 0} \frac{F_{\text{fall}} a_0 N_0 D^{0.5 + b_1 e - \lambda D}}{\int_{0}^{\infty} N_0 D^{3 + b_1 e - \lambda D} dD} = \frac{\int_{0}^{\infty} F_{\text{fall}} a_0 N_0 D^{b_1 e + 3} e^{-\lambda D} dD}{\int_{0}^{\infty} N_0 D^{3 + b_1 e - \lambda D} dD} = \frac{F_{\text{fall}} a_0 \sigma e_0 M_6}{a_0 \sigma e_0} M_0^{b_1 e/3} M_3^{b_1 e/3} = \frac{F_{\text{fall}} a_0 \sigma e_0 M_6}{a_0 \sigma e_0} M_0^{b_1 e/3} M_3^{b_1 e/3}.$$ (A8)

$$V_6 = \lim_{\rho \to 0} \frac{F_{\text{fall}} a_0 N_0 D^{b_2 e + 6 + \mu e - \lambda D}}{\int_{0}^{\infty} N_0 D^{6 + \mu e - \lambda D} dD} = \frac{\int_{0}^{\infty} F_{\text{fall}} a_0 N_0 D^{b_2 e + 6} e^{-\lambda D} dD}{\int_{0}^{\infty} N_0 D^{6 + \mu e - \lambda D} dD} = \frac{F_{\text{fall}} a_0 \sigma e_6 M_6}{a_0 \sigma e_6} M_0^{b_2 e/3} M_3^{b_2 e/3} = \frac{F_{\text{fall}} a_0 \sigma e_6 M_6}{a_0 \sigma e_6} M_0^{b_2 e/3} M_3^{b_2 e/3}.$$ (A9)

These expressions are identical to (27) and (28), respectively, in BOSS with $a_{p_2} = a_0 \sigma e_3$, $a_{p_3} = a_0 \sigma e_6$, $\tilde{b}_1 e_{p_2} = b_1 e_2 - d_6$, $\tilde{b}_2 e_{p_2} = b_2 e_1 - d_6$, $\tilde{b}_1 e_{p_3} = b_1 e_3 - d_6$, and $\tilde{b}_2 e_{p_3} = d_6$.

Similar to (A7), the quantities $X_{d3} = [\Gamma(4 + b v + \mu)/\Gamma(4 + \mu)]^{b_3 e/3}$ and $X_{d6} = [\Gamma(7 + b v + \mu)/\Gamma(7 + \mu)]^{b_3 e/3}$ are also approximated by single-term power expressions in the equations above, with parameters $\sigma e_3$, $\sigma e_6$, $d e_3$, and $d e_6$, obtained by directly fitting to $X_{d3}$ and $X_{d6}$ using least squares in log space. Values of the fitted parameters are shown in Table A4.

b. Condensation/evaporation

Below, we show how the condensation/evaporation rate in MORR can be expressed analytically in BOSS.
when ventilation is included but certain thermodynamic parameters are assumed constant. In section 3b, we show that ventilation effects in MORR can be well approximated using a single-term formulation for evaporation in BOSS with the “a" parameter increased by a factor of 5.

For gamma DSDs with μ = 0 in the two-moment MORR with prognostic M₀ and M₃ and neglecting ventilation effects, we obtain

\[
\left( \frac{dM_3}{dt} \right)_{\text{diff}} = \int_0^\infty F_{\text{diff}} N_0 D e^{-\lambda D} dD = F_{\text{diff}} 6^{-1/3} M_0^{2/3} M_3^{2/3},
\]

(A10)

using (A1) for λ and (A2) for N₀. This is identical to the single-term two-moment power expression in BOSS given by (12) with \(a_k = 6^{-1/3}\) and \(\beta_k = 1/3\).

The expression for the change in M₀ in MORR assumes the relative change in M₀ is proportional to the change in M₃. This gives

\[
\left( \frac{dM_0}{dt} \right)_{\text{diff}} = F_{\text{diff}} 6^{-1/3} M_0^{5/3} M_3^{-2/3},
\]

(A11)

which is identical to (12) in BOSS with \(a_k = 6^{-1/3}\) and \(\beta_k = 1/3\).

Similarly, for prognostic M₃ and M₆ we obtain

\[
\left( \frac{dM_3}{dt} \right)_{\text{diff}} = F_{\text{diff}} 120^{2/3} 6^{-1/3} M_0^{2/3} M_3^{-3/3} M_6^{2/3},
\]

(A12)

which is identical to (12) in BOSS with \(a_k = 120^{2/3}/6\) and \(\beta_k = -2/3\). The change in M₆ is proportional to the relative change in M₃. This gives

\[
\left( \frac{dM_6}{dt} \right)_{\text{diff}} = F_{\text{diff}} 120^{2/3} 6^{-1/3} M_0^{2/3} M_3^{2/3} M_6^{1/3},
\]

(A13)

which is identical to (12) in BOSS with \(a_k = 120^{2/3}/6\) and \(\beta_k = 1/3\).

For prognostic M₀, M₃, and M₆ in MORR-3MOM, the rain evaporation parameters are specified using gamma DSDs. This gives for the change in M₃,

\[
\left( \frac{dM_3}{dt} \right)_{\text{diff}} = \int_0^\infty F_{\text{diff}} N_0 D^{1+\mu} e^{-\lambda D} dD = F_{\text{diff}} \frac{\Gamma(2 + \mu)}{\Gamma(1 + \mu)} \frac{\Gamma(1 + \mu)}{\Gamma(4 + \mu)} M_0^{2/3} M_3^{2/3}
\]

\[
\approx F_{\text{diff}} \sigma_d \left( \frac{M_0 M_6}{M_3^2} \right)^{d_d} M_0^{2/3} M_3^{2/3} M_6^{1/3} = F_{\text{diff}} \sigma_d M_0^{2/3 + d_d} M_3^{-2/3 - 2d_d} M_6^{d_d},
\]

(A14)

which is identical to (13) in BOSS with \(a_k = \sigma_d\), \(\beta_{1,k} = -2/3 - d_d\), and \(\beta_{2,k} = d_d\). The change in M₆ is

\[
\left( \frac{dM_6}{dt} \right)_{\text{diff}} = F_{\text{diff}} \sigma_d M_0^{2/3 + d_d} M_3^{-2/3 - 2d_d} M_6^{d_d+1},
\]

(A16)

which is identical to (13) in BOSS with \(a_k = \sigma_d\), \(\beta_{1,k} = 1/3 - d_d\), and \(\beta_{2,k} = d_d + 1\).

When ventilation effects are included in MORR, the expressions for condensation/evaporation are identical to the BOSS formulation in (11) using two terms in the sum (\(L = 2\)), assuming \(\rho_a\) (kg m⁻³) and Schmidt number \(S_c = \mu_a/\rho_a D_a\) are constants (\(\mu_a\) is the dynamic viscosity of air). We demonstrate this analytically for M₀ and M₃ as the prognostic moments. In MORR-2MOM, the condensation/evaporation rate including ventilation effects is given by
\[
\left(\frac{dM_k}{dt}\right)_\text{diff} = \int_0^\infty F_{\text{diff}} N_0 e^{-\lambda D} \left[ f_1 D + f_2 \left( \frac{a \rho_a}{\mu_a} \right)^{1/2} S_\infty^{1/3} D^{3/2+b/3} \right] dD
\]

\[
= F_{\text{diff}} N_0 \left[ \frac{f_1}{\lambda} + \frac{f_2 \left( \frac{a \rho_a}{\mu_a} \right)^{1/2} S_\infty^{1/3} \Gamma \left( \frac{5}{2} + b/3 \right)}{\lambda^{3/2+b/3}} \right] \]

\[
= F_{\text{diff}} \left[ 6^{-1/3} f_1 M_0^{2/3} M_3^{1/3} + 6^{-1/2-b/6} f_2 \left( \frac{a \rho_a}{\mu_a} \right)^{1/2} S_\infty^{1/3} \Gamma \left( \frac{5}{2} + b/2 \right) M_0^{1/2-b/6} M_3^{1/2+b/6} \right],
\]

(A17)

where \( f_1 = 0.78 \) and \( f_2 = 0.308 \) following (Pruppacher and Rasmussen 1979). This is identical to (11) in BOSS using two terms in the sum, with \( L = 2 \). \( \alpha_{1,k} = 6^{-1/3} f_1 \), \( \alpha_{2,k} = 6^{-1/2-b/6} f_2 (a \rho_a/\mu_a)^{1/2} S_\infty^{1/3} \Gamma (5/2 + b/2) \), \( \beta_{1,1,k} = 1/3 \), and \( \beta_{1,2,k} = 1/2 + b/6 \). Here we assume constant \( \mu_a^{0.46} \mu_a^{-1} \) and \( S_c \) based on the domain average values from the tests described in section 3: \( \mu_a^{0.46} \mu_a^{-1} = 578.55.6 \) kg m\(^{-0.54} \) min\(^{-0.38} \) s and \( S_c = 0.5959 \). Also, \( \rho_a^{0.46} \mu_a^{-1} \) and \( S_c \) vary only 2.4% and 0.1%, respectively, across the domain in these tests. For the change in \( M_0 \) for two-term evaporation, the \( a \) parameters are the same as above, while \( \beta_{1,1,k} = -2/3 \) and \( \beta_{1,2,k} = -1/2 + b/6 \). The formulations using \( M_3 \) and \( M_6 \) as the prognostic moments are also exact with (11) in BOSS using two terms (again assuming constant \( \mu_a^{0.46} \mu_a^{-1} \) and \( S_c \)). Using \( M_0, M_3 \), and \( M_6 \) gives the same form as (11) with two terms when \( X_a \) is fit to a power expression similar to the three-moment derivation neglecting ventilation (not shown for brevity).

c. Collision–coalescence and collisional breakup

Expressions for collision–coalescence and collisional breakup in MORR, which are combined together in a single process rate equation calculation with a mean drop size–varying collection–breakup efficiency (Morrison et al. 2012), cannot be expressed in the BOSS framework analytically using one or two terms. This is because the MORR collision–coalescence–breakup formulation involves an exponential function of the mean drop size, which itself depends on the ratio of prognostic moments. Exponential functions can only be represented exactly via power series using an infinite number of terms. Nonetheless, the single-term drop–drop interaction process formulations in BOSS following (12) and (13) provide similar results to MORR, as described in section 3b. Consistent with MORR, BOSS parameter values are obtained based on the idea that equilibrium DSDs have a number-weighted mean diameter \( D_{Neq} = 6.0 \times 10^{-4} \) m, for which collision–coalescence and breakup are in approximate balance. Keep in mind that collision–coalescence rates for \( M_k \) are negative for \( k < 3 \) and positive for \( k > 3 \), whereas breakup rates are negative for \( k > 3 \) and positive for \( k < 3 \), as discussed in section 2. This adds a physical constraint for the sign of \( a_{k,\text{coal}} \) and \( a_{k,\text{break}} \).

For M0-M3-B, we chose values for \( a_{0,\text{coal}}, a_{0,\text{break}}, \) and \( \delta_{0,\text{coal}} \) for the simulations herein based on ad hoc testing of a small number of parameter values. The value of \( \delta_0 \) for collisional breakup is determined by

\[
\delta_{0,\text{break}} = \delta_{0,\text{coal}} + \frac{\log(-a_{0,\text{coal}}) - \log(a_{0,\text{break}})}{\log(6D_{Neq}^3)},
\]

(A18)

Equation (A18) ensures that the collisional breakup and collision–coalescence rates for \( M_0 \) are exactly equal in magnitude and opposite in sign when \( D_N = (M_3/6M_0)^{1/3} = D_{Neq} \), consistent with the concept of equilibrium DSDs. This expression for \( D_N \) as a function of \( M_0 \) and \( M_3 \) is valid for inverse exponential DSDs, consistent with the DSDs assumed by MORR.

Similarly for M3-M6-B, values of \( a_{6,\text{break}}, \delta_{6,\text{break}}, \) and \( a_{6,\text{coal}} \) for the simulations herein were chosen based on ad hoc testing of a small number of parameter values, with

\[
\delta_{6,\text{coal}} = \delta_{6,\text{break}} + \frac{\log(-a_{6,\text{break}}) - \log(a_{6,\text{coal}})}{\log(120D_{Neq}^3)},
\]

(A19)

Equation (A19) ensures that collisional breakup and collision–coalescence rates for \( M_6 \) are exactly balanced when \( D_N = (M_6/120M_3)^{1/3} = D_{Neq} \).

For M0-M3-M6-B, parameters for the change in \( M_0 \) from collision–coalescence and collisional breakup follow those for M0-M3-B for simplicity. Consistent with MORR-3MOM, parameters for the change in \( M_6 \) from collision–coalescence and breakup are specified such that \( M_6M_6/M_3^3 \) is constant (see Table A3). Taking \( d(M_0M_3M_6^{-2})/dt \) implies \( (dM_0/dt)_{\text{coal}} = -(M_0/M_0)(dM_0/dt)_{\text{coal}} + (dM_0/dt)_{\text{break}} = -(M_0/M_0)(dM_0/dt)_{\text{break}} \).


