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DECOVALEX-2019: An international collaboration for advancing the understanding and modeling of coupled thermo-hydro-mechanical-chemical (THMC) processes in geological systems

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ABSTRACT

The DECOVALEX Project is an international research collaboration for advancing the understanding and modeling of coupled thermo-hydro-mechanical-chemical (THMC) processes in geological systems. DECOVALEX stands for "DEvelopment of COupled Models and VALidation against EXperiments". The creation of this international initiative, now running for almost 30 years, was motivated by the recognition that prediction of these coupled effects is an essential part of the performance and safety assessment of geologic disposal systems for radioactive waste and spent nuclear fuel, and also for a range of other sub-surface engineering activities. DECOVALEX emphasizes joint analysis and comparative modeling of state-of-the-art field and laboratory experiments, across a range of host rock options and repository designs. Participating research teams are from radioactive waste management organizations, national research institutes, regulatory agencies, universities, and consulting groups, providing a wide range of perspectives and solutions to these complex problems. The most recent phase of the DECOVALEX Project, here referred to as DECOVALEX-2019, started in 2016 and ended in 2019. Modeling teams from 13 international partner organizations participated in the comparative evaluation of seven modeling tasks involving complex field and/or laboratory experiments. This Virtual Special Issue on DECOVALEX-2019 provides an in-depth overview of these collaborative research efforts and how these have advanced the state-of-the-art of understanding and modeling coupled THMC processes.

1. Introduction

An important part of the performance and safety assessment of disposal systems for radioactive waste and spent nuclear fuel in deep geological formations is the evaluation of the impact of the coupled effects of mechanical deformation, fluid and gas flow through the repository, and thermal loading from the decaying waste. It was recognized early on in safety and performance assessments conducted for geologic disposal sites that to be able to conduct such an evaluation, there was a need to rigorously enhance the theoretical background and to develop models capable of simulating coupled thermo-hydromechanical (THM) processes. More recently, chemical (C) processes have also been added to enable the study of fully coupled THMC processes in geosystems.

The term "coupled processes" implies that each process potentially affects and is affected by the initiation and progress of other processes. Thus, the response of a rock mass to radioactive waste storage cannot be predicted with confidence by considering each process individually or in direct succession. In the field of rock mechanics and rock engineering, many studies have been made on two-way coupling (e.g., TM and HM), but for the repository performance problem, it is essential to study and be able to give reasonable assurance of the prediction of processes with THM coupling, and even full THMC coupling. Such coupling remains a major challenge to the science and engineering community, in part because relevant effects need to be better understood and described with constitutive relations, but also since the processes have widely different characteristic temporal and spatial scales. Coupled processes of course are not only relevant to geologic disposal of radioactive waste but also play a critical role in a range of other sub-surface engineering activities, such as carbon dioxide sequestration, enhanced geothermal systems, energy storage, as well as unconventional oil and gas production through hydraulic stimulation.

In 1992, recognizing the need to address the modeling challenges related to coupled THM and (in later stages) THMC processes, DECO-VALEX was initiated as an international cooperative project of nuclear waste organizations, including implementers, regulators, and research institutions, plus a large number of associated research and modeling teams, providing a wide range of perspectives and solutions to these

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complex problems (www.decovalex.org). Analysis and comparative modeling of state-of-the-art field and laboratory experiments has been at the core of the collaborative work, with an increasing focus on characterizing uncertainty and blind prediction of experimental results. Since 1992, the project has gone through several four-year phases, each phase featuring a number of selected modeling challenges of importance to radioactive waste disposal. Six project phases were successfully concluded between 1992 and 2015, results of which have been summarized in several overview publications (e.g. Refs.^{1–3}) and in a series of Special Issues in the International Journal of Rock Mechanics and Mining Sciences (Vol. 32(5) in 1995, Vol. 38(1) in 2001, and Vol. 42 (5–6) in 2005), in the Journal of Environmental Geology (Vol. 57(6) in 2009), and in the Journal of Environmental Earth Sciences (Virtual Topical Collection, 2016).

The 7th phase of the DECOVALEX project, here referred to as DECOVALEX-2019, comprised of modeling teams from 13 international partner organizations, which participated in the comparative evaluation of seven modeling tasks (i.e., Tasks A through G). Together, these tasks address a wide range of relevant issues related to engineered and natural system behavior in a variety of potential host rocks. The 29 publications in this Virtual Special Issue provide an in-depth overview of the collaborative research efforts conducted in each task and how these have advanced the state-of-the-art of understanding and modeling coupled THMC processes. Below, we briefly introduce each task, provide references to respective publications, and explore some common lessons learned that have emerged across the tasks. One of the most important characteristics of DECOVALEX is the emphasis on a cooperative research environment and the desire to gain insight by comparative analysis of multiple alternative approaches. This characteristic is reflected in this Virtual Special Issue by jointly authored synthesis papers for each task. These provide an overview of the modeling approaches pursued by individual research teams and discuss which concepts and models have been particularly suited for a given coupled problem. The synthesis papers are supplemented by more detailed publications describing the research methods and findings of individual teams.

2. DECOVALEX-2019 tasks

The seven DECOVALEX-2019 tasks can be grouped into the four following general themes:

- Novel Representations of Micro-Scale Processes (Tasks A and F)
- THM Processes in Clay-Based Materials (Tasks D and E)
- Modeling Coupled Processes in Complex Fracture Networks (Tasks C and G)
- Complex Hydro-Mechanics with Relevance for Broader Subsurface Engineering Applications (Task B)

The tasks under each theme are discussed below.

2.1. Novel representations of micro-scale processes

2.1.1. Task A: ENGINEER - modeling advective gas flow in low permeability sealing materials

The purpose of Task A was to better understand the processes governing gas migration in low permeability clay-based barrier materials (Fig. 1). Special attention was given to the fundamental mechanisms and controlling factors for gas migration, such as gas entry and flow, or pathway stability and sealing, which will affect barrier performance. The modeling task utilized a series of well-instrumented small-scale laboratory experiments that were conducted by the British Geological Survey (BGS). Task participants tested new model concepts in comparison to a variety of tests that were conducted under different conditions and dimensionalities, including 1D and pseudo-spherical gas flow at constant volume and constant stress. Eight international modeling teams participated in ENGINEER using four types of modeling approaches: (i) standard two-phase flow models incorporating a range of different mechanical deformation behaviors. (ii) enhanced two-phase flow models in which fractures are embedded within a plastic material (continuous techniques) or incorporated into the model using a rigid-body-spring network (discrete approaches), (iii) a single-phase model incorporating a creep damage function in which only gas flow is considered, and (iv) a conceptual approach used to examine the chaotic nature of gas flow. A summary of the collaborative research work conducted in this DECOVALEX task is given in the synthesis paper by Tamayo-Mas et al.⁴ Detailed results from individual modeling groups can be found in Chittenden et al.⁵; Dagher et al.⁶, Damians et al.⁷; Kim et al.⁸; and Harrington et al.9

2.1.2. Task F: FINITO - fluid inclusion and movement in the tight rock

The purpose of this modeling task was to refine and compare modeling approaches for the behavior of fluid inclusions in tight lowpermeability rock (Fig. 2). Fluid inclusions may be found within mineral crystals or along grain boundaries in evaporitic formations as well as in many sedimentary rocks and can migrate in the presence of thermal or hydro-mechanical gradients. For the disposal of radioactive waste, common host rock candidates such as clay and salt rock are considered tight with respect to fluid movement and such fluid inclusions are typically stagnant. However, they may become mobilized by a perturbation of the in situ state, which can occur due to excavation and other geotechnical installations, the emplacement of heat-generating waste, or the generation of gas pressure. The migration of fluid inclusions can have important impacts on the long-term performance of a geologic repository for high-level radioactive waste disposal. Task F was designed to investigate two aspects of fluid inclusion migration in rock salt under different boundary conditions: (a) altered hydro-mechanical conditions as a consequence of tunnel excavation or borehole drilling and (b) coupled thermo-hydro-mechanical-chemical conditions during the heating period in the post-closure phase of a repository. The three teams involved in this task collaborated to improve process understanding and



Fig. 1. Conceptual model of gas flow under different conditions for porous media.¹⁰



Fig. 2. Halite grain boundaries with fluid inclusions.¹²

model concept development. Aspects of the research work conducted in Task F are given in Shao et al. 11

2.2. THM processes in clay-based materials

2.2.1. Task D: INBEB - hydro-mechanical (HM) and THM Interactions in Bentonite Engineered Barriers

The objective of INBEB (Interactions in Bentonite Engineered Barriers) was the interpretation and modeling of the performance of an initially inhomogeneous bentonite barrier, based on data from two fullscale long-term experiments. These are the isothermal Engineered Barrier (EB) experiment (Fig. 3), which ran for over ten years at the Mont Terri URL, and the non-isothermal FEBEX heater test, which was in operation for more than 18 years at the Grimsel Test Site. In both cases, a comprehensive post-experiment dismantling and characterization effort provided uniquely detailed three-dimensional information of the bentonite barrier properties at the end of each test. INBEB assessed the evolution from a newly installed unsaturated engineered system to a fully functioning barrier, using HM and THM model predictions in comparison to the experimental data. Special attention was paid to the evolution of barrier heterogeneity under transient conditions and on the final state reached upon saturation. This requires improved constitutive relationships to describe material behavior and properties in hydrating bentonite, an enhanced understanding of the fundamental processes that lead to barrier homogenization, and improved capabilities for modeling coupled HM and THM processes in complex geo-materials. Four international research teams participated in INBEB. In general, the numerical models were able to represent adequately the trends in the observed TH



Fig. 3. Picture shows EB Experiment in construction. A dummy canister sits on a bed of compacted bentonite blocks. The pipes for the artificial hydration system of the bentonite are visible.¹³

and THM behavior modelled. A summary of the collaborative research work conducted in this task is given in the synthesis paper of Gens et al.¹³ Further details from individual teams are given in Lee et al.¹⁴; Takayama¹⁵; and Michalec.¹⁶

2.2.2. Task E: upscaling of heater test modeling results

The purpose of this modeling task was to evaluate upscaling approaches for THM modeling in the Callovo-Oxfordian (COx) claystone host rock, starting with small size experiments (some cubic meters) to real scale emplacement cells (some ten cubic meters) all the way to scale of a waste repository (cubic kilometers). To achieve this aim, Task E utilized data from in-situ heating experiments performed by Andra (the French National Radioactive Waste Management Agency) in the Meuse/ Haute-Marne Underground Research Laboratory (MHM URL). The repository design developed by Andra assumes that waste canisters are placed horizontally in parallel micro-tunnels drilled from access drifts. A comprehensive research program was conducted in the Meuse/Haute-Marne URL near Bure to investigate the THM response of the COx to thermal loading from these microtunnels, through laboratory and in-situ experiments. The *in-situ* experimental program consists of a step-by-step approach ranging from small-scale heating boreholes (TED experiment) to a full-scale experiment of a single emplacement tunnel (ALC experiment - Fig. 4). Task E started with modeling of the TED experiment to derive THM parameters by means of a calibration exercise and then used these parameters for a blind prediction of the ALC experiment. As a final modeling step, the models tested against the ALC data were extrapolated to a model for the entire repository with multiple emplacement tunnels. Five teams participated in Task E. A summary of the collaborative research work conducted in this Task is given in two synthesis papers, the first by Seyedi et al.¹⁷ on upscaling from the TED to the ALC heater tests, the second by Plua et al.¹⁸ on intercomparison of approaches to model the entire repository. Additional information on individual modeling efforts is given in Plua et al.¹⁹; Bumbieler et al.²⁰; Guo et al.^{21–23}; Wang et al.^{24,25}; Thatcher et al.^{26,27}; Xu et al.²⁸; and Yu et al.²⁹

2.3. Modeling coupled processes in complex fracture networks

2.3.1. Task C: GREET - modeling hydro-mechanical-chemical-biological processes during groundwater recovery in crystalline rock

Task C centered on the GREET test, a full-scale experiment recently conducted in the Japanese Mizunami URL (crystalline rock) to evaluate the natural resaturation of the near-field environment of a geologic repository after repository closure (Fig. 5). GREET stands for Groundwater REcovery Experiment in a Tunnel. The goals of GREET were as follows: (1) to understand the water recovery processes and mechanisms of the near-field fractured rock, (2) to verify coupled hydrological-mechanical and chemical simulation methods for modeling these processes, and (3) to develop monitoring techniques for the facility closure phase and appropriate closure methods taking recovery processes into account.



Fig. 4. Three-dimensional layout of the ALC experiment.²⁰



Fig. 5. Schematic of the GREET experiment (based on³⁰; and.³¹).

The primary features of interest to be modelled in Task C were the water pressure drawdown and recovery, and the variation of water chemistry during the tunnel excavation and closure, as observed in the monitoring boreholes and the closure test drift (CTD) itself. Three modeling teams used a range of deterministic and stochastic approaches to represent how high-permeability fracture pathways near the tunnel impact groundwater recovery and water chemistry. Once et al.³⁰ and Hokr & Balvin³¹ describe modeling activities conducted for DECOVALEX Task

C.

2.3.2. Task G: EDZ evolution: reliability, feasibility, and significance of measurements of conductivity and transmissivity of the rock mass

The formation and evolution of the excavation disturbed and excavation damage zone (EDZ) around deposition tunnels and holes is an important topic in the development of radioactive waste disposal concepts. In crystalline host rock, the formation of an EDZ will increase the transmissivity of the rock mass in the vicinity of the excavations and thus raise the potential for fluid migration parallel to the excavations. Task G was primarily concerned with modeling the evolution of EDZ transmissivity throughout the lifetime of a repository from construction to pre-closure and post-closure phases. A secondary focus was on the challenges and uncertainties for monitoring rock mass permeability as a function of time during construction and operation of a repository hosted in fractured crystalline rock. The task was based on detailed EDZ transmissivity tests performed in the TAS04 tunnel in the Äspö Hard Rock Laboratory in Sweden (Fig. 6). A summary of the collaborative research work conducted in this DECOVALEX task is given in Meier and Backers³² and modeling of fracture transmissivity changes in response to excavation, thermoshearing, and glaciation is presented in Kwon and Min³³.

2.4. Complex hydro-mechanics with relevance for broader subsurface engineering applications

2.4.1. Task B: modeling the induced slip of a fault in argillaceous rock

This modeling task evaluated the conditions for slip activation and stability of faults in clay formations, with focus on the complex coupling between fault slip, pore pressure, permeability creation, and fluid migration. This subject is of great importance to many subsurface applications where injection of fluids leads to pore-pressure increase and reduction of effective normal stress on faults, which in turn can cause fault reactivation. Regarding radioactive waste emplacement, increases in pore pressure could be due to release of heat from the high-level waste or the generation of gas due to metal corrosion. The possibility of an



Fig. 6. Positions of drill holes in the floor of the TAS04 drift, plotted based on coordinates given in Appendix 1 of Ericsson et al.³⁴ Note that the vertical scale in this view is exaggerated.

increased permeability caused by fault slip is of concern for the longterm safety of a repository. The central element of this Task B was the FS Fault Slip Experiment conducted in the Mont Terri Underground Research Laboratory in Switzerland, which utilized a novel experimental setup for controlled fault slip testing in a realistic underground setting at field scale (Fig. 7). Six modeling teams participated in this task, using both interface approaches or solid finite elements to account for the fault discontinuity. In general, the hydromechanical behavior of the fault as observed in the field was captured best as a propagating rupture along an existing weakness plane with damage-enhanced permeability. A summary of the collaborative research work conducted in this DECOVALEX task is given in the synthesis paper by Rutqvist et al.³⁵; with further details provided in Park et al.³⁶ and Shiu et al.³⁷

3. Main achievements and remaining challenges

DECOVALEX-2019 successfully explored some common themes across a range of complex modeling tasks (see further discussion of themes below), yielding new insights but also encountering common issues that remain to be resolved. Significant progress was achieved by research teams of all tasks. Modeling teams adopted advanced modeling approaches using different numerical methods and computer codes and were generally able to achieve good agreement, both compared to the experimental observations and compared to other teams using alternative modeling approaches. In cases where differences remain, task leads and modeling teams made efforts to isolate the reasons for them and discussed what could be done to improve. Overall, the achievements and outstanding issues obtained from the seven tasks form an important step forward for better understanding of the scientific/technical issues of importance for safe geological disposal of radioactive wastes in different host rocks, with complex geological conditions and increasing environmental challenges.

3.1. Novel representations of micro-scale processes

Both Tasks A and F both dealt with fundamental challenges in



Fig. 7. (A) Three-dimensional view of the Mt Terri Main Fault plane with the location of the FS experiment; (B) Simplified cross section of the Main Fault with the blue rectangles indicating the location of the packed-off sections; (C) SIMFIP test equipment setup; (D) Schematic view of the three-dimensional deformation unit. Tubes are differently colored to show that they display different deformations when there is a relative movement of the rings anchored to the borehole wall across the activated fracture.³⁸ (For interpretation of the references to color in this figure legend, the reader is referred to the Web version of this article.)

understanding and modeling the highly non-linear fluid migration observed in very low permeability formations. Observed experimental and field behaviors are often strongly stochastic and therefore it can be very difficult to rationalize the core physical behavior (i.e., identify what experimental features are reproducible under different circumstances) and successfully interpret the experiments. In addition, the experimental setup can be very important in determining the result, hence careful representation of the experiment (e.g., explicit representation of the injector apparatus used in the laboratory experiments in Task A) can be key to building a successful model. In this context, the DECOVALEX working model of close integration between experiment and modeling is an important one. In Task A, the primary concern was the migration of pressurized gas in compacted bentonite, while Task F mainly considered migration of inclusions in salt formations. While superficially quite distinct, there are a number of commonalities. For Task A, it was shown that conventional two-phase flow approaches are largely inadequate to represent the observed behavior, taking into account all the known features of the experimental results (e.g., very low gas saturations at breakthrough). Hence the inclusion of implicit or explicit features to represent the dilation process is essential. Similarly, for Task F, explicit treatment of fluid migration along the halite grain boundaries, also by a dilation process under strongly deviatoric stress conditions, was found to be a good representation of salt inclusion migration. Both tasks illustrated the importance of micro-scale control on macro-scale phenomena and novel approaches for bringing the micro-scale understanding into the meso- and macro-scale have been put forward.

3.2. THM processes in clay-based materials

Tasks D and E considered HM and THM processes in clays or claybased materials such as bentonite or clay, at the waste disposal scale. Task E demonstrated that good blind predictions of pore-pressure and temperature can be obtained for heat-generating disposal analogs using thermal diffusion models with conventional elastic poro-mechanics. There was some evidence of surprising local heterogeneity in the clay at the MHM URL which meant some recalibration was required when moving between experiments, illustrating the potential impact of variability and heterogeneity on pore pressure. The teams were also able to upscale their models to represent the whole repository, and use these models to investigate the sensitivity of uncertainty and variability on key metrics (pore pressure and implied effective stress) that could impact the safety case. In understanding the details of the experiments, it was clear that the development of the EDZ, and the resulting effective hydraulic and mechanical properties of the EDZ, were important to calibrate the models to the observations. While the task demonstrated a generally good representation of scale-dependent THM processes, the treatment of mechanical damage and the resulting change in the clay properties remain areas of significant uncertainty. Task D focused on compacted and pelleted bentonite used as a clay-based buffer material. While teams were also able to obtain good agreement with the measured thermal and hydraulic responses, a complete representation of the plastic deformation - in this case focused on the homogenization of the bentonite during heating and resaturation - remained challenging. Hence both tasks encountered similar issues in terms of the treatment of the plasticity of clays, albeit from different perspectives (homogenization in Task D, induced damage in Task E). These issues with damage/ plasticity represent the major uncertainties in the work to date and hence areas for future investigation to improve the robustness of understanding.

3.3. Modeling coupled processes in complex fracture networks

Tasks C and G both dealt with the problem of interpreting groundwater flows and (in the case of Task C) transport within discrete fracture networks (DFNs) in crystalline host rock. This is an area of long-standing study within DECOVALEX and the tasks have encountered many of same

issues, albeit from a different perspective. Both tasks illustrated that realistic DFN models, based on geological observation, can successfully represent net tunnel inflows after some calibration. Some teams were also successful when using an equivalent continuum porous medium (EPCM) approach rather than a DFN model. However, both tasks ran into modeling challenges when looking at more complex aspects of the problem. In the case of Task C, successfully modeling the wide range of observed chloride concentrations in the tunnel was particularly problematic. Producing a convincing representation of the transport required manual intervention in the DFN/EPCM to connect the excavated tunnel to vertically distant higher and lower concentrations of chloride. Task G showed a similar issue at a much smaller scale, whereby the interference tests in the TAS04 experiment were very hard to interpret and model when using intersections of planar fracture surfaces identified in the EDZ. Both tasks concluded that channelization with the fracture network could be the cause of the difficulties in modeling the observations, noting that large scale heterogeneities in the DFN network for Task C could also be a factor.

3.4. Complex hydro-mechanics with relevance for broader subsurface engineering applications

Task B focused on an individual fault zone in a low-permeability claystone rather than DFN systems in a crystalline potential host rock as discussed above. Modeling teams addressed numerical challenges associated with fluid injection and reactivation in a fault system with a complex structure comprising of a strongly foliated fault core enveloped by a fractured damage zone. The task used data from a highly instrumented in situ test which provides valuable insights into the complex relationship between pressure buildup, fault opening, fault slip, and fluid migration. The collaborative modeling work in Task B clearly illustrated the numerical complexities of simulating complex discontinuous features experiencing normal and shear displacement under hydraulic control. Different numerical methods were found to have contrasting strengths and weaknesses in representing the highly nonlinear nature of the hydro-mechanical response. Extensive work on an initial benchmarking exercise provided coherence between the modeling tools and gave good confidence that the basic couplings were being represented properly. However, large differences were seen between modeling approaches in more complex cases where plastic damage on shear features is suspected to play an important role. This has parallels with the DFN work where the presence of stochasticity is important. Task B is of interest outside of the radioactive waste management arena, being of direct relevance to other sub-surface engineering applications (e.g., geologic carbon sequestration, geothermal energy, underground energy storage, etc.).

4. Conclusions

The results of the collaborative modeling in DECOVALEX-2019 have produced some clear outcomes and common issues across a diverse portfolio of complex modeling task. There have been considerable successes in moving forward the science of predicting coupled processes in geological materials, but there remain non-trivial issues that are of direct relevance to a wide range of geo-engineering applications.

The work has shown that true blind predictions remain one of the best methods of building confidence in modeling approaches. Success has been had in low permeability systems predicting THM responses. However, it is necessary to consider the input uncertainty when making predictions, especially if outcomes of interest are broadly linear (e.g., pressure response) whereas the key uncertainties and log-normally distributed (e.g., intrinsic permeability). Significant progress has also made in modeling advective movement of gas in clays, with a range of 1D/2D/3D models being used successfully to give a reasonable representation of the experimental observations. It is clear from this work that a conventional continuum multi-phase flow representation of gas

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migration is not an appropriate method; rather alternative approaches or major augmentations of existing methods are required to produce physically plausible models. This is an area of ongoing research which is being continued in the ongoing DECOVALEX-2023 Project phase.

Science challenges around stochasticity were felt in several tasks. The time-series stochastic features in some experimental observations cause considerable difficulties in attempting to represent the experiment using essentially deterministic models. While it can be argued that a stochastic system should be modelled using a stochastic model, when only single or small numbers of experiments are available, modelers are effectively forced to use deterministic representations to understand the fundamental processes, with the treatment of the observed stochasticity a future research area. Some success was achieved using chaotic representations to understand such data, but these methods are very much in their infancy. A few modeling teams also tackled the reverse problem where stochastic models were used to condition against deterministic data for fractured rock representations. From this work there was clear evidence that details of flow and transport are not well represented using parallel plate square or circular fractures; channels or pipes appear necessary to explain experimental observations.

The representation of HM processes in large fracture systems was generally successful, but there was a heavy divergence in results dependent on the details of the numerical method used. This makes application of these models in a predictive mode difficult and the results subject to considerable uncertainty. In addition, the representation of plasticity and damage in clay rocks remains a key uncertainty and is difficult to model as an emergent phenomenon.

We hope that the brief summary presented above, and the in-depth research findings in the selected papers, provide an idea of the breadth and depth of cutting-edge research work carried out within the DECOVALEX-2019 project. With this Virtual Special Issue, we also intend to convey to interested readers the value of the DECOVALEX philosophy of cooperation between international researchers of different disciplines using a range of different approaches. Such collaboration means frequent interactions, sharing of data and results, collectively generating new ideas and concepts, raising technical issues in joint communications, and performing critical reviews of each other's work. The insight obtained in such integrated cooperative efforts would have been impossible if the teams had worked independently. Comparison of model results with other international modeling groups, using their own simulation tools and conceptual understanding, enhances confidence in the robustness of predictive models used for performance assessment. In addition, the possibility of linking model differences to particular choices in conceptual model setup provides valuable guidance into "best" modeling choices and understanding the effect of conceptual models on predictions.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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