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Reply to comment by Flewelling and Sharma on "Hydraulic fracturing in faulted sedimentary basins: Numerical simulation of potential contamination of shallow aquifers over long time scales"

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1. Introduction

We welcome and appreciate the comments of *Flewelling and Sharma* [2015, hereafter referred to as FS] which give us the opportunity to clarify and discuss important aspects of our study [*Gassiat et al.*, 2013, hereafter referred to as G13]. FS discuss some important details of the model development and implementation of G13. The main thrust of FS is that parts of the model geometry, parameters and boundary conditions are inappropriate, and model calibration is insufficient for a specific shale gas basin, the St. Lawrence basin. However, the work of G13 was fundamentally a parametric study, using data from multiple shale gas basins to define model geometry, parameters and boundary conditions, and the objective was not to robustly calibrate results to a specific shale gas basin. Below we systematically address the specific comments of FS about the limitations of G13, which provide us an opportunity to further elaborate on the already extensive discussion of such limitations in G13 [paragraphs 36–47].

The objectives of G13 were to assess if hydraulic fracturing could lead to contamination of shallow aquifers via preferential fluid migration along faults, and what factors control the potential for significant contaminant transport into shallow aquifers. As described in G13, the objectives were met by: (1) compiling publically available data on shale gas formations, fault parameters, and hydraulic fracturing operations; (2) using a numerical model to simulate the effect of shale gas fracturing in a generic faulted sedimentary basin with properties that are representative of the compiled data; and (3) conducting a sensitivity analysis with the model to examine the sensitivity of fluid flow along a fault to different parameters, including basin, fault, and hydraulic fracturing parameters that cover the range of literature values.

G13 is part of a larger research effort trying to address the question of whether fluids migrate to shallow aquifers from hydraulically fractured shales over long time periods and degrade groundwater quality. FS have themselves considered this question by looking at the potential for fluid migration through the bulk of a stratigraphic column [*Flewelling and Sharma*, 2013; *Flewelling et al.*, 2013]. FS have made significant scientific contributions to this issue, although these contributions have also been criticized [*Rozell*, 2014; *Flewelling and Sharma*, 2014]. Instead, G13 considered fluid migration through preferential fluid flow paths, namely permeable faults. Fluid migration along preferential flow paths has been considered as a potentially significant groundwater contamination process by all major national inquiries on the potential environmental impacts of shale gas development [*Bureau d'audiences publiques sur l'environnement (BAPE)*, 2011; *US EPA*, 2012; *The Royal Society and The Royal Academy of Engineering (RS and RAE)*, 2012; *Ewen et al.*, 2012; *Jackson et al.*, 2013; *Soeder et al.*, 2014; *Council of Canadian Academies (CCA)*, 2014; *Comité de l'évaluation environnementale stratégique sur le gaz de schiste (CÉES)*, 2014]. Contrary to what FS suggest, numerous scientific studies provide much more than anecdotal evidence of the importance of fluid flow along faults [see references in G13 as well as in review papers *Garven*, 1995; *Faulkner et al.*, 2010; *Bense et al.*, 2013]. In fact, the importance of better understanding this process and its potential environmental impacts was taken seriously enough to initiate scientific studies by national research agencies in the United States [*US Environmental Protection Agency*, 2012] and Canada (Geological Survey of Canada) [*Lavoie et al.*, 2014; *Rivard et al.*, 2014]. Furthermore, the USA EPA study has already lead to major developments in numerical simulation capabilities that would allow the investigation of some of the processes that were mentioned, but not fully considered in G13 [*Moridis and Freeman*, 2014; *Freeman et al.*, 2013; *Kim and Moridis*, 2013; *Rutqvist et al.*, 2013].

2. Model Set Up

We agree with FS that there needs to be more attention paid to ensuring that models that simulate the potential environmental effects of hydrofracturing are reasonably realistic. To our best knowledge, no study has yet simulated the potential environmental impacts of hydrofracturing on aquifers with a full representation of all processes involved: multiphase system, density-dependent flow, reactive mass transport and hydromechanical effects. This is essential and will be done in the near future [*US EPA*, 2012] but this is a daunting numerical task with significant technical and computing challenges, not to mention parameterization requirements. As part of the studies carried out thus far, a simple analytical analysis, such as the one of *Flewelling and Sharma* [2013], is useful for scoping of processes. The numerical analysis of *Rutqvist et al*. [2013] is also of much interest as it deals with fault re-activation, but it does not address fluid flow. Contrary to the suggestion of FS, neither of these references provides a realistic analysis of the potential long-term environmental impacts of hydrofracturing via existing regional-scale faults. There is thus a need for initial numerical studies, such as G13, that assess how fluid flow could occur along permeable faults in relation with hydrofracturing.

Contrary to the implicit interpretation made by FS, the purpose of G13 was not to investigate a specific sedimentary basin. Rather, the purpose of G13 was to investigate the processes related to fluid flow along a permeable fault and to independently evaluate the potential contamination using the best publically available data and models available at the time of research. G13 synthesized publically available data from multiple shale gas basins (G13 Table 1). Disclosure of data held by the petroleum industry data would help the development of conceptual as well as numerical models and their parameterizations. The emphasis placed on the St. Lawrence basin and the Utica Shale was due to the more readily available set of properties for that sedimentary basin and the familiarity of authors with the area, although the model geometry, parameters and boundary conditions of G13 are generally consistent with other shale gas basins.

Another important clarification, also potentially misinterpreted by FS, is that G13 did not attempt to assess the likelihood of fluid flow along permeable faults, but rather to identify the set of conditions and parameters that would favor potential fluid flow along a fault. G13 makes no claim that the conditions identified as leading to more fluid flow along a fault are likely to occur in any given sedimentary basin. Modeling using specific conditions of a given study area would have to be used to assess if fluid migration is likely to occur along preferential paths, such as done for south-eastern Germany [*Lange et al*., 2013; *Kissinger et al*., 2013].

2.1. Fault Representation and Constraints on Fluid Overpressure

The geometry of the pre-existing, through-going fault simulated by G13 is consistent with regional-scale faults in the St. Lawrence basin and other regions with shale gas exploitation. The question of the extent of faults through the overlying shales is uncertain in some sedimentary basins as imaging of steeply dipping faults is intrinsically difficult with available seismic techniques. For example, geological cross sections of *Séjourné et al*. [2013] depict some continuous faults to surface but the seismic data acquired in the St. Lawrence basin were aimed to image the deep units under the Utica, which makes the shallow data of poor quality. Despite this uncertainty on fault extent in the St. Lawrence basin, since G13 is a generic process study, we assume the presence of such continuous faults and examine their potential effects on fluid flow. Since the hydraulic continuity of regional-scale faults remains uncertain, we explicitly evaluated this in the sensitivity analysis which included both fault permeability as well as fault anisotropy.

As discussed by FS, fractures in shales are often self-healing but regional-scale faults cross-cutting shale horizons are not just composed of shale, but rather could have complex fault architectures including fault cores, damages zones, fault juxtaposition, clay smears, etc. [*Bense et al*., 2013; *Caine et al*., 1996]. Without detailed basin-specific data on fault zone hydrogeology it is difficult to establish the hydraulic continuity of a fault zone, which is why we approached this problem as a parametric sensitivity analysis. FS question the "probability" of specific conditions. Although this is a welcome discussion, the objective of G13 was to evaluate the "potential" for fluid migration.

FS argue that it is not possible to have both a highly permeable fault and persistent overpressure. This assertion is contradicted by numerical results from G13, that show a small region of reduced overpressuring in shale at the fault (G13 Figure 4a), although this still leads to upward fluid movement driven by the pressure of the shale. Furthermore, we used two numerical modeling periods that involve an initialization period (300,000 years) to allow flow and pressures to reach near steady state conditions, and a second period (100,000 years) to confirm that near steady state conditions were achieved. Simulations showed that the initial equilibration period did not lead to a significant dissipation of overpressure. The overpressure is maintained in the model in the shale simply because of its low permeability. The shale cannot depressurize over a significant distance also due to its low permeability. This result contradicts the analytical result of FS. One significant difference between the model and the analytical solution is that the model represents water flow whereas the analytical solution was applied to gas flow. The very different viscosities of water compared to gas may be a factor leading to these contradictory results.

Even though the assumption that overpressures are maintained after shale gas production may appear simplistic, it could be envisioned that such conditions would occur if the volume of the shale in contact with fractures created by hydrofracturing represents a small proportion of the overall shale volume, gas recovery is small (a few %) and long-term gas overpressures are recovered through slow processes, such as diffusion, from the intact shale into the induced fracture network. The fact that a second (or more) hydrofracturing operation can lead to renewed shale gas production provides an indication that the initial gas pressure was not depleted by the first stage of production. However, conditions leading to the stopping or restarting of commercial shale gas production are controlled by many factors besides the pressure state of the gas, which does not have to be overpressured to allow gas production. We recognize the importance of this issue and the need for further work, especially since G13 numerical modeling results have shown the importance of overpressure for fluid migration along a permeable fault. Such further work should not be limited to the prediction of the gas pressure state immediately following production, but would have to consider the processes that could act in the long-term that could influence gas pressure recovery. Furthermore, such work would benefit from data on pressure conditions after shale gas production.

As mentioned in G13 and FS, the simulations in G13 do not consider multiphase processes that would be required to fully represent the fluid and gas migration. The multiphase processes involved in fluid migration are complex as they could either promote or limit fluid migration, and therefore further research is required. For example, one could also presume that the presence of gas bubbles in the fluid column within a fault could lead to an overall light fluid column and enhance its buoyancy and overall upward migration, similar to gas lift in oil wells that brings upward not only gas but also liquids (both oil and brine). New numerical capabilities are just emerging to represent such near-field multiphase processes [*Moridis and Freeman*, 2014; *Freeman et al*., 2013; *Kim and Moridis*, 2013].

We agree with FS that terminating the fault in the base of the shale at a prescribed no flow boundary necessarily leads to upward rather than downward fluid flow, which could be important if the permeability of the underlying formation is large and is at a lower pressure than the overlying shale. For the assessment of the potential for fluid flow along faults in a specific basin, we thus agree that both flow directions would have to be considered. For the specific case of the St. Lawrence basin, FS mention that flow could be downward from the Utica Shale. However, *Tran Ngoc et al*. [2014] show that deep saline aquifers in that basin can also be overpressured, whereas *Chatellier et al*. [2013] show that overpressured conditions start even in the units above the Utica Shale. This being said, for a process study such as G13 it is not unreasonable to assume overpressure and only upward flow. FS also state that the Utica Shale could also seal the fault. Although possible, that would not change G13 modeling results since it is the increased permeability induced by hydrofacturing on the top portion of the shale that leads to upward flow along the fault. So whether the fault is permeable or not within the shale is not an important point for the model used.

Overall, on the issues discussed in this section, the arguments of FS regard mostly whether or not the conditions used in the model adequately represent the specific conditions encountered in the St. Lawrence Basin, which misses the purpose of G13.

2.2. Aspects of Oil and Gas Operations

We have mentioned in G13 and previously in this reply that we consider the proper representation of the "near-field" related to the horizontal well and its surrounding fractured shale as a major control on the potential migration of fluids from fractured gas shales. G13 made a number of simplifying assumptions regarding the fractured shale as the proper representation of the near-field source term would require efforts that were beyond the scope of G13.

FS identify limitations in the representation made of oil and gas operations in G13 and provide calculations to support their arguments. However, the FS calculation presented in that section assumes that the entire shale is depleted. As mentioned previously, we would rather consider that the overpressure would be maintained at least partly by lateral migration into the produced zone in the long-term. Also, FS refer to *Senger et al*. [1987] to support their assertion that pressure will deplete in the gas shales and that overpressure will not be reestablished before thousands of years. We would argue that this reference does not represent an appropriate analog for gas shales. First, the argument made by G13 was that gas production through hydrofracturing of the shale would not be "complete," which is supported by the very low proportions of gas in place reported as recoverable from gas shales. G13 thus assumed that the gas shale would remain overpressured even after commercial gas production. Furthermore, this process is quite distinct from production of conventional reservoirs as reported by *Senger et al*. [1987] for which the cause of overpressure is the presence of a hydrocarbon column in a reservoir, whereas overpressure in a gas shale is related to the incapability for the formed gas to escape the shale. It follows that conventional reservoirs cannot be used as analog to represent the processes of depressurization of gas shales. A more appropriate analog for pressure equilibration in shales could be found in the work of *Tóth and Corbet* [1987] who have calculated equilibration times between 0.1 and 10 million years for pressures to adjust to land erosion in a shale at different depths. This work does not indicate to what extent overpressure could remain in hydrofractured and produced shales, but it shows that any remaining overpressure would persist for a very long time.

2.3. Permeability and Recharge

The low recharge rate used in the model actually has no significant impact on results since G13 did not use concentrations in the aquifer as indications of impact potential but rather the fluxes and concentrations of solutes reaching the base of the aquifer. Since fluid circulation in the units overlying the gas shale does not play a significant role, lowering their permeability as suggested by FS would not change the results of G13 appreciably. Actually larger permeability values in this unit would allow higher recharge in the aquifer. However, we agree with FS that if the impact on the aquifer was assessed then recharge would be an important parameter for future analysis.

The analytical solution presented by FS in the permeability and recharge section appears sound, but it leads to unrealistic results, likely in part because the solution does not include density-dependent flow and brine distribution as G13 do. Saline water is known to occur at depths beyond 200 m and even during glacier melting the 200 m deep "recharge" is an appropriate depth [*Person et al*., 2012]. So the model was set up to have an "active" groundwater flow zone coherent with the known flow zone as mentioned before. The theoretical 4500 m depth of the active flow zone obtained by FS is totally in contradiction with observations, not only in the St. Lawrence basin but other basins as well. Active flow depends more on topography, this is what drives groundwater flow deep. Even then, the higher permeability near surface restricts the flow in the upper part [*Tóth*, 1963; *Jiang et al*., 2009; *Laurencelle et al*., 2013].

3. Model Consistency

Although not discussed in G13 due to space limitations, the model simulated the depth intervals at which waters having different salinity ranges are found in the St. Lawrence and other sedimentary basins. More specifically, simulations consistently represented the thickness of the low salinity groundwater found in the active near-surface flow zone, which is typically on the order of a couple of hundred meters below the surface. For typical permeability values of the aquifer system, recharge was then specified at a value leading to an active flow zone of about 200 m. The thickness of this active flow zone is also controlled by the topography and imposed heads at the top surface of the model. The legend in Figure 4b of G13 is correct but misleading in that the red colour shows a concentration greater than 0.1, with most of the values below approximately 200 m being $C = 1$, which FS correctly interpreted as concentration of 100 kg/m^3. Therefore, the model simulations are consistent with the salinity conditions in the St. Lawrence basin and other sedimentary basins.

As stated above, the purpose of G13 was not validation or calibration of the generic model, but to understand the settings and processes that may potentially be important for solute migration along a permeable fault. These goals were achieved through parametric simulations and sensitivity analysis. G13 thus uses a common parametric simulation approach of local sensitivity analysis where properties are individually and systematically modified over a reasonable parameter range to assess their relative effects on fluid flow along a permeable fault. The base case for numerical modeling and the range of changes made to properties were based on a thorough literature review in order to use representative and plausible parameters. Model studies across diverse but related fields such as hydrogeology, petroleum engineering, contaminant hydrogeology, and watershed hydrology often take a similar parametric approach, starting with some of the earliest groundwater studies through to present day [e.g., *Tóth et al.*, 1963; *Freeze and Witherspoon*, 1967; *Winter*, 1976; *Gomez and Wilson*, 2013; *Pasala et al.*, 2013]. To this end, even the utility of model validation or calibration in the hydrologic sciences has been of much debate [e.g., *Oreskes et al.*, 1994; *Konikow and Bredehoeft*, 1992].

4. Shale Tracer

We acknowledge that the simulated tracers were conservative and that results shown by G13 on tracer migration represent a worst case scenario. We agree with FS that to study the potential migration of specific contaminants, degradation and retardation processes would have to be considered. Although not a health issue, the migration of conservative species, such as chloride, would contribute to the degradation of groundwater quality and could even limit its use. This being said, since predicted concentrations following migration were not used to assess the potential impact of fluid migration, the transport process does not have significant impact on the conclusions of G13. In G13, mass transport was used in the form of tracers to identify the origin and destination of fluids flowing along a permeable fault. However, we agree that the assessment of potential impacts on a specific aquifer, especially for specific contaminants, would have to consider degradation, retardation, and ion-exchange processes in addition to the specific geochemical conditions of a given basin. Furthermore, fluid flowing along a permeable fault could gain or lose some geochemical components, which could mitigate or worsen the effect of fluid migration to a superficial aquifer.

5. Conclusions

We reiterate that the purpose of G13 was to numerically simulate salient features of a generic regional-scale fault system in order to evaluate their potential role in environmental impacts of hydrofracturing. Despite the limitations that were already recognized and described by G13, as well as those pointed out by FS, we argue that G13 used the best publicly available data to define reasonable model geometry, parameters and boundary conditions. We thus consider that the main conclusion of G13 stands: fluid migration along permeable faults from hydrofracturing zones is plausible under some specific conditions and thus needs to be considered, and that assessment has to consider a long-term time frame. G13 is one contribution of a larger research effort evaluating if fluids could migrate to shallow aquifers from hydraulically fractured shales over long time periods and degrade groundwater quality. We look forward to vigorous and ongoing scientific discussion and to additional research addressing this important topic in the near future.

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