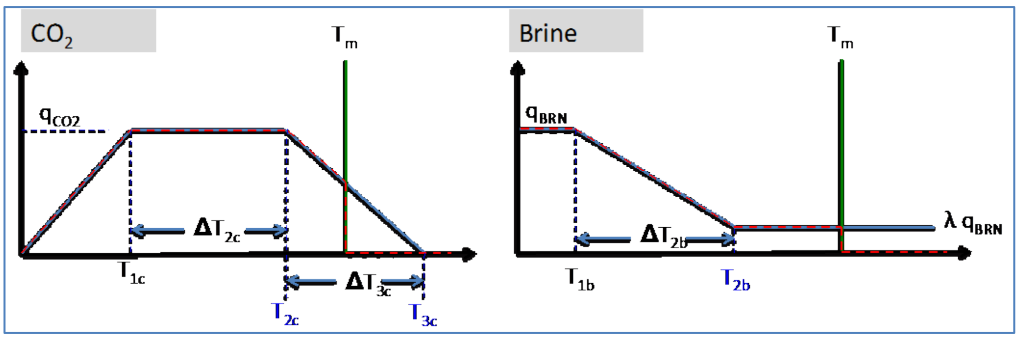

Development of a General Form CO_2 and Brine Flux Input Model

11 April 2017

Office of Fossil Energy

NRAP-TRS-III-019-2017

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Cover Illustration: Schematic of the High Plains Aquifer and changes in groundwater pH from CO_2/brine leakage.

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Development of a General Form CO_2 and Brine Flux Input Model

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Acronyms, Abbreviations, and Symbols

Term	Description
λ	Ratio of brine leakage tail
ΔT	Difference between two consecutive time periods
CO_2	Carbon dioxide
DOE	U.S. Department of Energy
LLNL	Lawrence Livermore National Laboratory
M_{BRN}	Mass of brine
M_{CO2}	Mass of CO_2
NRAP	National Risk Assessment Partnership
NUFT	Non-Isothermal, Unsaturated and Saturated Flow and Transport Code
PSUADE	Computer code of Problem Solving environment for Uncertainty Analysis and Design Exploration
q_{BRN}	Maximum brine flux
q_{CO2}	Maximum CO_2 flux
R^2	Linear Correlation Coefficient
ROM	Reduced-order model
T_{1b}	Time to maximum brine flux
T_{2b}	Time to initial decrease in brine flux
T_{1c}	Time to maximum CO_2 flux
T_{2c}	Time to initial decrease in CO_2 flux
T_{3c}	Time to zero CO_2 flux
TDS	Total dissolved solids
UQ	Uncertainty quantification

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ABSTRACT

The National Risk Assessment Partnership (NRAP) project is developing a science-based toolset for the quantitative analysis of the potential risks associated with changes in groundwater chemistry from carbon dioxide (CO_2) injection. In order to address uncertainty probabilistically, NRAP is developing efficient, reduced-order models (ROMs) as part of its approach. These ROMs are built from detailed, physics-based process models to provide confidence in the predictions over a range of conditions. The ROMs are designed to reproduce accurately the predictions from the computationally intensive process models at a fraction of the computational time, thereby allowing the utilization of Monte Carlo methods to probe variability in key parameters.

This report presents the procedures used to develop a generalized model for CO_2 and brine leakage fluxes based on the output of a numerical wellbore simulation. The resulting generalized parameters and ranges reported here will be used for the development of third-generation groundwater ROMs.

1. OBJECTIVE

The objective of this report is to detail the procedures used to develop a generalized model to represent carbon dioxide (CO_2) and brine leakage fluxes based on the output of a numerical wellbore simulation.

Implementation of a generalized flux model was proposed to encompass a large range of CO_2 and brine input fluxes propagated from a pressurized reservoir through a borehole. These generalized models facilitate the implementation of fluxes in an uncertainty quantification (UQ) framework since the relevant leakage rate and time parameters can be generated randomly. The basic shape for these models were constructed from the results of numerical wellbore simulations based on pressure and saturation profiles derived from the Kimberlina reservoir model Wainwright et al. (2013) coupled with wellbore permeability to yield CO_2 and complimentary brine leakage functions (Figure 1). The numerical simulations were based on 48 potentially vertical leaky wells located within 5,000 m of the CO_2 injection well in the High Plains Aquifer in Southwest Kansas (Carroll et al., 2014). Fluxes for each wellbore were simulated with 1,000 randomly generated wellbore permeability parameters to yield a total of 48,000 numerical simulations using the NUFT (Nitao, 1998) code. The resulting fluxes determined from this generalized approach will be integrated into an uncertainty quantification framework to statistically generate CO_2 and brine fluxes and subsequently implemented as elemental sources at a depth of 198 m to the bottom of a 10,000 m × 5,000 m × 240 m (x, y, z) numerical model with a variably spaced mesh consisting of 190,250 nodes (Carroll et al., 2014).

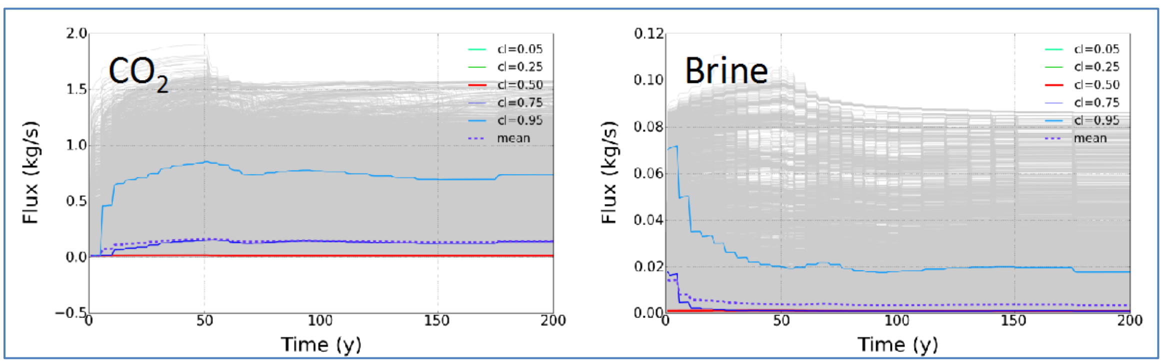

Figure 1: CO_2 and brine fluxes resulting from numerical wellbore simulations with confidence intervals. Grey lines on each plot represent one of 48,000 flux curves.

2. METHODOLOGY

The structure of the generalized flux models was based on the predominant structure of the numerical simulations, whereby CO_2 fluxes increase to a plateau then decrease after a sustained time period and brine fluxes decrease to rates less than the initial input flux. To test the comparison of the numerical and generalized fluxes, simple signal processing methods were applied to derive the peak CO_2 fluxes (q_{CO2}), the time to reach the peak (T_{1C}), the duration of the peak flux (ΔT_{2C}) and the duration to decrease (ΔT_{3C}), and the initial (q_{BRN}) and final (λq_{BRN}) brine fluxes and their transitionary periods (T_{1B} and ΔT_{2B}). An additional parameter will be included in the third-generation aquifer models to represent mitigation time (T_M). A conceptualized model of the generalized flux curves with parameters is shown in Figure 2.

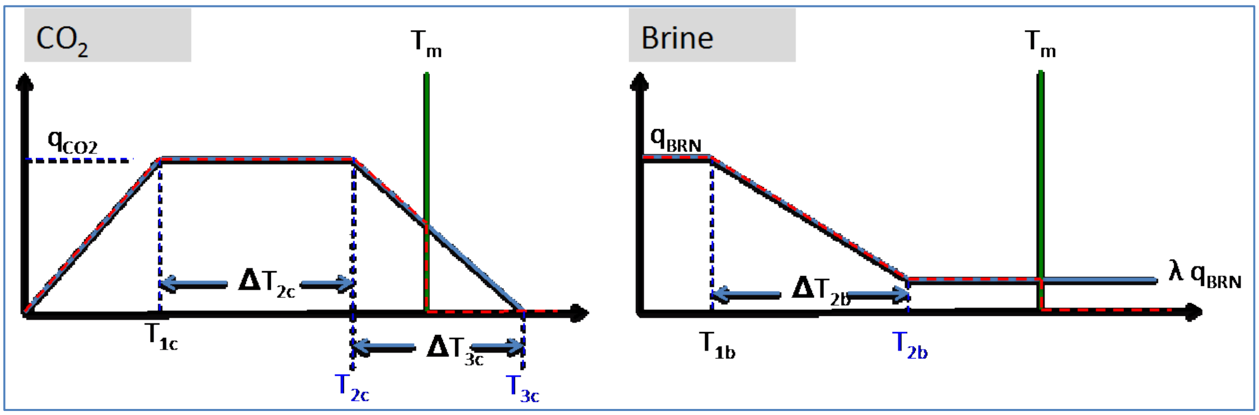

Figure 2: Basic shape of CO_2 (left) and brine (right) generalized input curves with parameters.

Conversion of the CO_2 input curves into a generalized form followed a few basic procedures. First, the input fluxes from the numerical simulations were smoothened using a two-pass filter to remove localized noise. The peaks were estimated by calculating the second derivative of the curve to estimate q_{CO2} and ΔT_{2c}. Curves with single peaks were assigned a minimum of 5 years to represent the duration of the peak flux (ΔT_{2C}). The CO_2 flux at 200 years for the generalized form was assigned the value of the input curve at 200 years. The cumulative mass is calculated by:

$$M_{CO2} = \frac{q_{CO2}\,(T_{1C})}{2} + q_{CO2}\,(\boldsymbol{\Delta} T_{2C}) \;+ \frac{q_{CO2} + q_{co2@200y}}{2}\;(200 - T_{2C}) \qquad (1)$$

Subsequently, the CO_2 flux (q_{CO2}) was optimized to match the cumulative mass of the input curve by the following:

$$q_{CO2-OPT} = \frac{M_{CO2} - \frac{q_{CO2@200y}(200-T_{2C})}{2}}{\frac{T_{1C}}{2} + \Delta T_{2C} + \frac{(200-T_{2C})}{2}} \qquad (2)$$

The optimized mass was calculated by substituting $q_{CO2-OPT}$ into Equation 1. Use of the generalized form allows for efficient computation and implementation of the optimized flux and it captures the key processes observed from the numerical wellbore simulations.

Figure 3 shows four random examples from 1,000 emulations selected from wellbores 3, 10, 20 and 35 of CO_2 input flux curves converted into non-optimized and optimized general form.

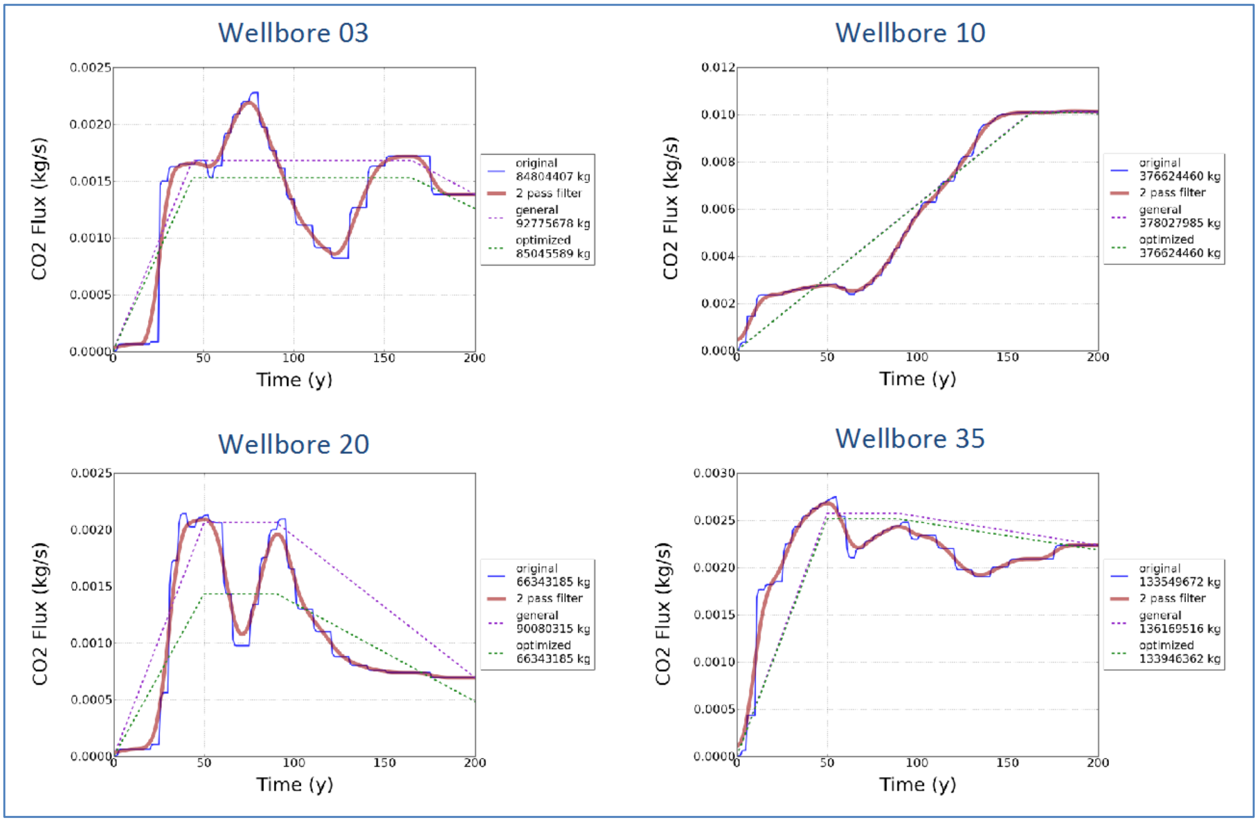

Figure 3: Randomly selected CO_2 input curves from numerical situations converted into a non-optimized and optimized general form input function using Equation 2.

Generalized parameters for the brine input curves were calculated creating a coarse 3 bin histogram of the input fluxes to average the initial (q_{BRN}) and tail (λq_{BRN}) fluxes, then determining the duration of the initial flux (T_{1B}) based on the time length of the average initial flux and calculating the transition time between the two fluxes ($\mathbf{\Delta} T_{2B}$) by calculating the start period (T_{2B}) for the tail flux. The cumulative mass is calculated by:

$$M_{BRN} = q_{BRN}\,(T_{1B}) + \frac{(q_{BRN}) + (\lambda q_{BRN})}{2}\,(\mathbf{\Delta} T_{2B}) + \lambda q_{BRN}\,(200 - T_{2B}) \qquad (3)$$

To match the cumulative mass from the input curve, and optimized tail flux value was estimated by:

$$\lambda q_{BRN-OPT} = \frac{M_{BRN} - q_{BRN}\,(T_{1B}) - \frac{q_{BRN}(\Delta T_{2B})}{2}}{\frac{\Delta T_{2b}}{2} + (200 - T_{2B})} \quad (4)$$

The optimized mass was calculated by substituting $\lambda q_{BRN-OPT}$ into Equation 1.

Examples of randomly selected brine flux curves converted into non-optimized and optimized general form are shown in Figure 4 from wellbores 3,10, 20 and 35 (from 1,000 samples for each wellbore).

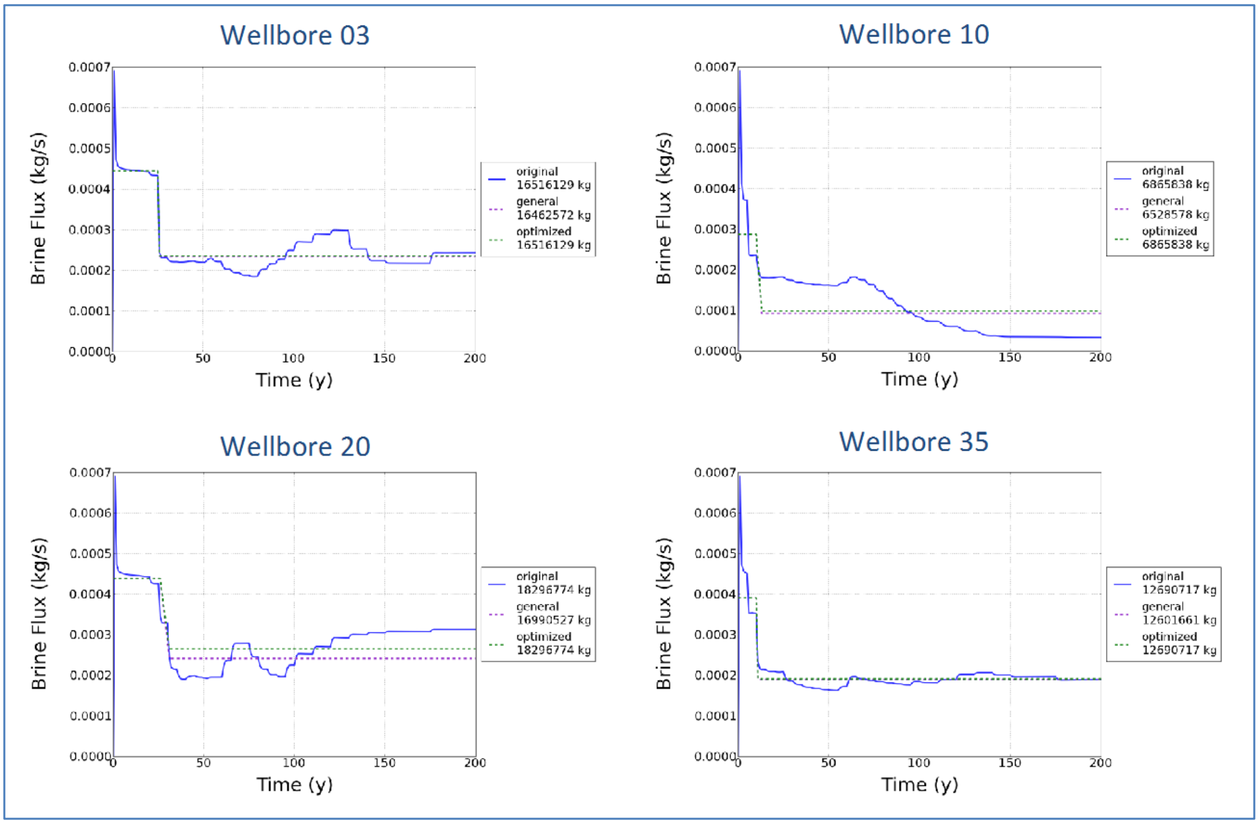

Figure 4: Randomly selected brine input curves from numerical situations converted into a non- optimized and optimized general form input curve using Equation 4.

3. RESULTS

Figure 5 shows the accuracy of the conversion process by comparing cumulative fluxes resulting from the numerical simulations and converted general form. Cumulative mass of CO_2 and brine was selected since these are the most sensitive parameters for groundwater impact (Carroll et al., 2014). Both fluxes result in close agreement between the two non-optimized models based on the high correlation coefficient (R^2) values.

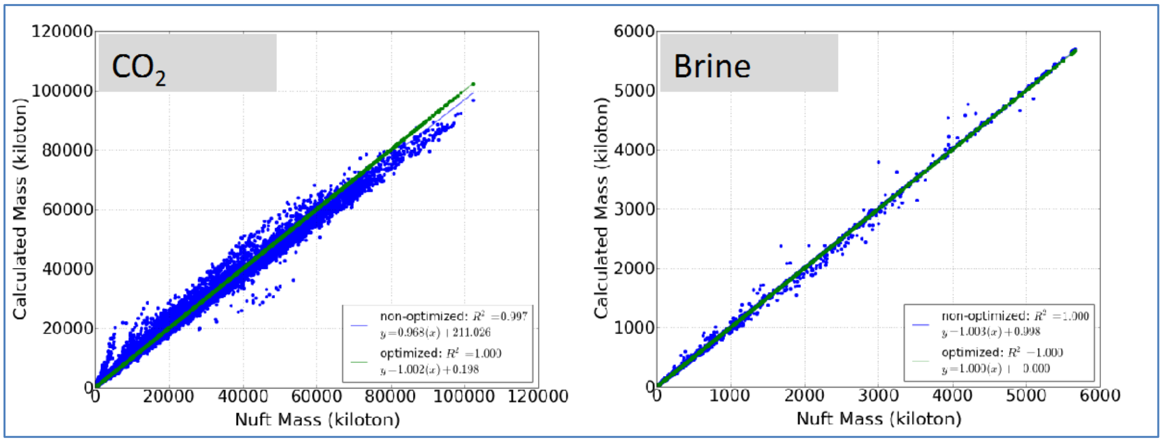

Figure 5: Comparison of cumulative CO_2 (left) and brine (right) mass computed from the numerical models and generalized models. Each graph compares 48,000 data points based on non-optimized mass (blue dots) and optimized mass (green dots).

Parameter ranges for the generalized model were derived from the conversion of the numerical simulations into the generalized form by analyzing the parameter distributions derived from the conversions based on numerical wellbore simulations. A list of the parameters and ranges are detailed in Table 1.

Table 1: Proposed parameter ranges for generalized CO_2 and brine leakage models

Parameter	Min	Max	Notes
q_{CO2}	-3.0	-0.301	Log10 (0.001–0.5) kg s^{-1}
q_{BRN}	-3.0 (-2.301)	-1.125	Log10 (0.005–0.075) kg s^{-1}
λ	0.2	0.300	Ratio of brine-leakage tail to q_{BRN}
T_{1c}	5.0	50.000	yr
ΔT_{2c}	0.0	100.000	yr
ΔT_{3c}	5.0	50.000	yr
T_{1b}	1.0	50.000	yr
ΔT_{2b}	1.0	10.000	yr
T_m	50.0	200.000	Mitigation time, yr

The resulting CO_2 and brine flux curves based on the generalized model with parameters populated from Table 1 is presented in Figure 6.

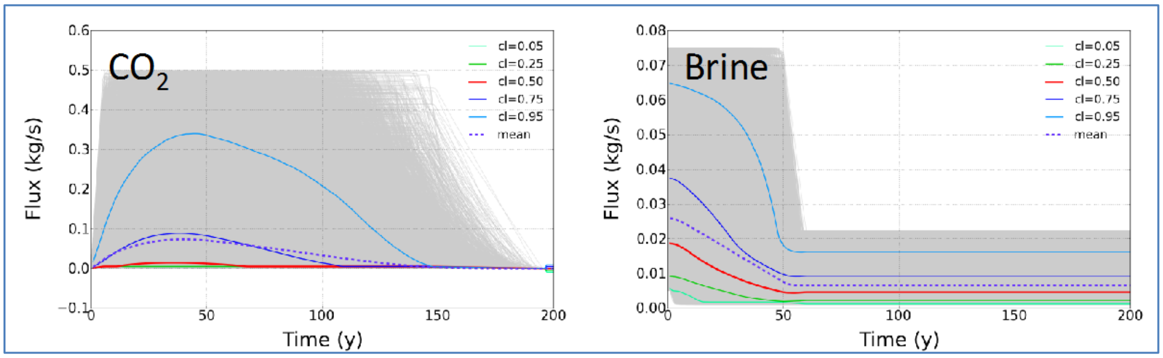

Figure 6: Randomly generated CO_2 and brine fluxes for generalized model applying the parameter ranges listed in Table 1. Grey lines on each plot represent one of 48,000 flux curves. Mitigation time is omitted.

4. SUMMARY

In summary, it is demonstrated that a generalized model representing the input fluxes for CO_2 and brine can be a simplified model that mimics the behavior of the numerical model. It is important to note that the generalized model does not consider location or proximity to the injection well, which can affect the behavior of the flux. However, this approach can be adapted to represent a broad range of input fluxes and easily adapted into a UQ framework.

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NRAP is an initiative within DOE's Office of Fossil Energy and is led by the National Energy Technology Laboratory (NETL). It is a multi-national-lab effort that leverages broad technical capabilities across the DOE complex to develop an integrated science base that can be applied to risk assessment for long-term storage of carbon dioxide (CO_2). NRAP involves five DOE national laboratories: NETL, Lawrence Berkeley National Laboratory (LBNL), Lawrence Livermore National Laboratory (LLNL), Los Alamos National Laboratory (LANL), and Pacific Northwest National Laboratory (PNNL).

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