May 12, 2011

MEMORANDUM TO: Christepher A. McKenney, Chief
Performance Assessment Branch
Environmental Protection
and Performance Assessment Directorate
Division of Waste Management
and Environmental Protection
Office of Federal and State Materials
and Environmental Management Programs

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SUBJECT: TECHNICAL REVIEW: MODELED RELEASE OF TECHNETIUM USING SIMPLE GOLDSIM MODELS, DOCKET NO. PROJ0734

The U.S. Nuclear Regulatory Commission (NRC) staff has created a series of GoldSim models to assess the modeled release of technetium-99 from a grout monolith (enclosed). The calculations described in this document are scoping calculations intended to demonstrate the performance of various modeling approaches.

Enclosure:
Onsite Observation Guidance

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Modeled Release of Technetium using Simple GoldSim Models

May 9, 2011

The U.S. Nuclear Regulatory Commission (NRC) staff created three simple GoldSim models to assess the modeled release of Technetium-99 (Tc-99) from a grout monolith. The release and transport of Tc-99 is sensitive to its oxidation state. Tc-99 is retained under reducing conditions and is highly mobile under oxidizing conditions. The calculations described in this document are scoping calculations intended to demonstrate the performance of various modeling approaches. The selection of particular parameter values should not be interpreted as an endorsement of these parameter values by the NRC staff.

The GoldSim model created by NRC staff has three submodels: a *one cell* model, a *two cell* model, and a *ten cell* model.

one cell submodel: In this model, the entire grout monolith was represented by *one cell* in GoldSim. The sorption coefficient, or K_d value, assumed for this cell was a weighted average of the oxidized and reduced K_d values based on the fraction of the monolith that is oxidized. As an example, if the grout monolith was modeled as being 5% oxidized then the cell would have an effective K_d value that is 95% of the reduced K_d value or 950 mL/g.

two cell submodel: In this model, the grout monolith was represented using two cells, an oxidized cell and a reduced cell. The sorption in the oxidized cell was represented by the oxidized grout K_d and the sorption in the reduced cell was represented by the reduced grout K_d.

ten cell submodel: The *ten cell* model is similar to the *two cell* model, but in this submodel the reduced and oxidized regions are each represented by five cells in series.

These simple models only include advective flow. Diffusive fluxes out of the wasteform were not considered. Solubility limits were not included in the models, and the cells were assumed to be fully saturated (i.e., the cells only contain grout and water).

The grout wasteform is assumed to have a density of 1000 kg/m^3 and a porosity of 0.6. The grout monolith is assumed to have a width of 200 ft (60.96 m), a length of 600 ft (182.88 m), and a height of 25 ft (7.62 m). In the *two cell* and *ten cell* models, the volume of grout in the oxidized and reduced cells was determined by multiplying the entire volume of the monolith by the assumed oxidized and reduced fractions. A value of 0.1 mL/g was assumed for the K_d, of technetium in the oxidized grout and a value of 1000 mL/g was assumed for the K_d of technetium in the reduced grout. An inventory of 100 Ci of technetium was assumed for the entire monolith in the models.

The calculations were performed for three different types of flow: slow flow, fast flow, and mixed flow. In the slow flow calculation, an advective flow rate of 7.8 m^3/yr was assumed to go through the grout monolith. This flow was based on an assumed hydraulic conductivity of 2.22e-9 cm/s and the area of the monolith. In the fast flow calculations, an advective flow of 3345 m^3/yr was assumed to go through the grout monolith. This was based on an assumed infiltration rate of 30 cm/yr and the area of the monolith. In the fast flow case, it is assumed that the grout is degraded enough to transmit all of the infiltrating water through it. In both the slow and fast flow calculations for the *two cell* and *ten cell* models, the flow rate described above is the total flow rate through the grout. The flow rates through the oxidized and reduced cells were determined by multiplying the total flow rate by the fraction that is oxidized or reduced. In the mixed flow calculations, it was assumed that the oxidized portion of the monolith is also degraded, while the reduced portion of the monolith is intact. Therefore, in these calculations the slow flow rate was assumed for the reduced portion of the grout, and the fast flow rate was assumed for the oxidized portion. In the *one cell* submodel, the mixed flow calculations used a weighted average of the fast and slow flow values based on fraction of the monolith assumed to be oxidized.

The following graphs show the flux of Tc-99 from the grout monolith and the total fraction of Tc-99 released calculated using the three different models. The fluxes presented in the graphs below represent the total advective flux from the monolith. For the *two cell* and *ten cell* models, this corresponds to the sum of the flux from the oxidized and reduced cells. The calculations were performed assuming various oxidized fractions as well as the three different types of flow. The fraction that was oxidized was assumed to remain constant with time, which is a simplification of the behavior expected in the real system. In the real system, it is expected that the fraction of the wasteform that is oxidized would increase with time. As can be seen from the graphs below, the calculated fluxes and fractional releases in the *one cell* model are not consistent with the results calculated using the *two cell* and *ten cell* models, except in the cases where a very small fraction of the monolith is oxidized. Furthermore, even in cases in which the total fraction of technetium leached during the 10,000-year period of interest is similar, the peak flux of technetium predicted by the 2 and 10 cell models can be significantly greater than the flux modeled by the *one cell* model. This difference in flux is significant because the peak flux typically directly affects the peak dose. In many cases, the peak fluxes from the *one cell* model are orders of magnitude less than from the *two cell* and *ten cell* models. This is especially true for the mixed flow calculations. In some cases, the fluxes and/or fractional releases from the different models converge at later times. This is a modeling artifact due to the simplifying assumption that the fraction of the wasteform that is oxidized remains constant with time. As a result, in these models the oxidized portion of the wasteform becomes quickly depleted of technetium, and at later times the release from the wasteform is driven by the release from the reduced portion of the wasteform. This behavior is not expected in the real system because the fraction of the real system that is oxidized would increase over time.

The results of these calculations indicate that modeling the flux out of the grout monolith using a single weighted K_d value can significantly under predict technetium leaching, as compared to a more detailed model, under many flow and oxidation conditions.

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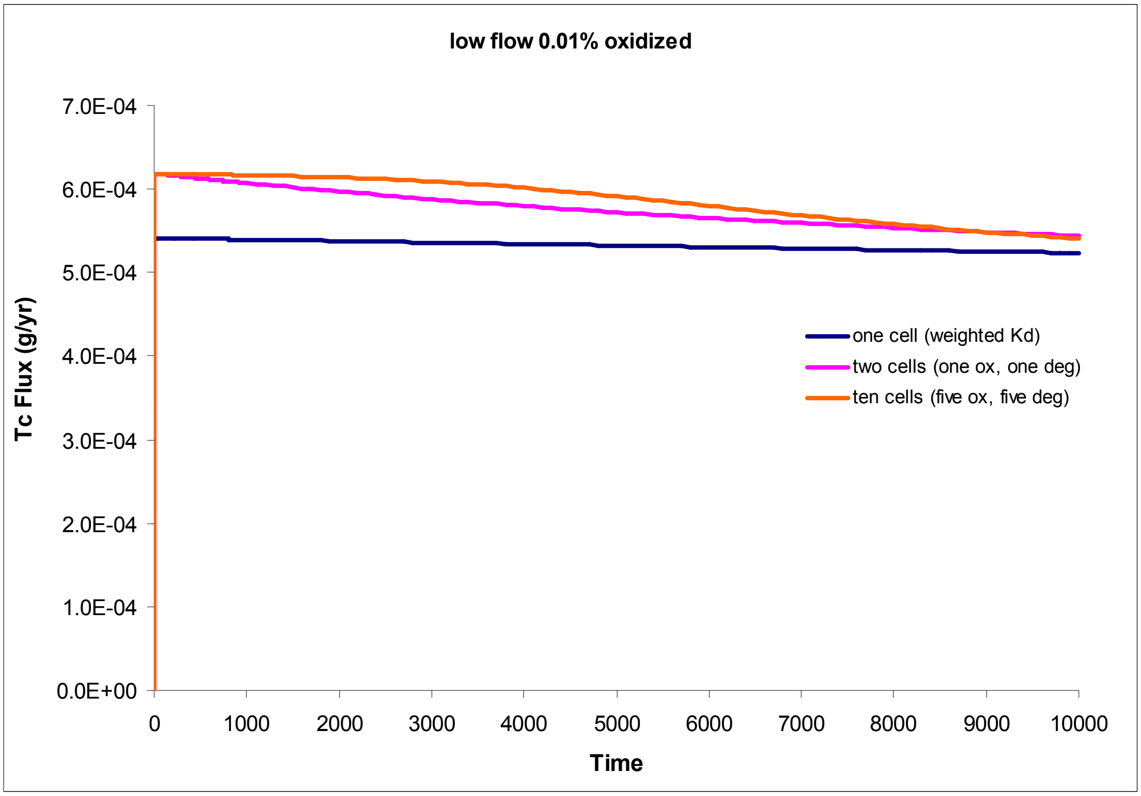


Figure 1: Modeled Tc flux from grout assuming 0.01% oxidized and low flow

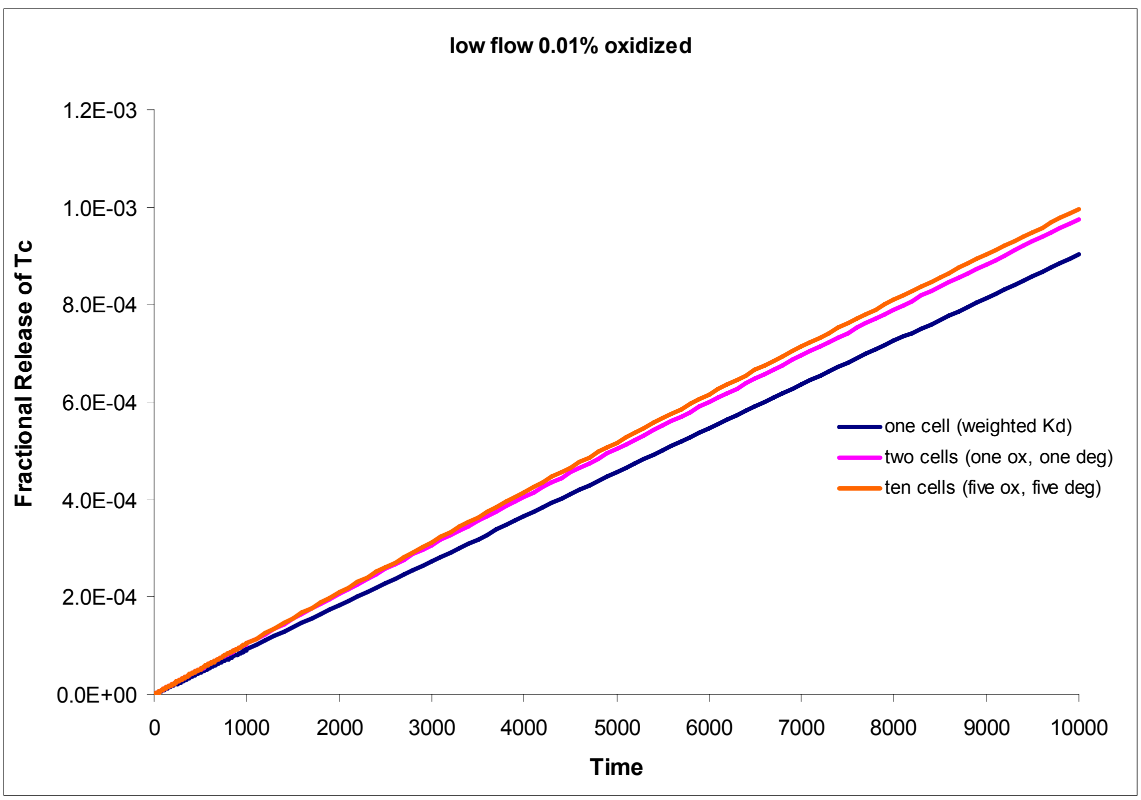


Figure 2: Cumulative fractional release of Tc assuming 0.01% oxidized and low flow

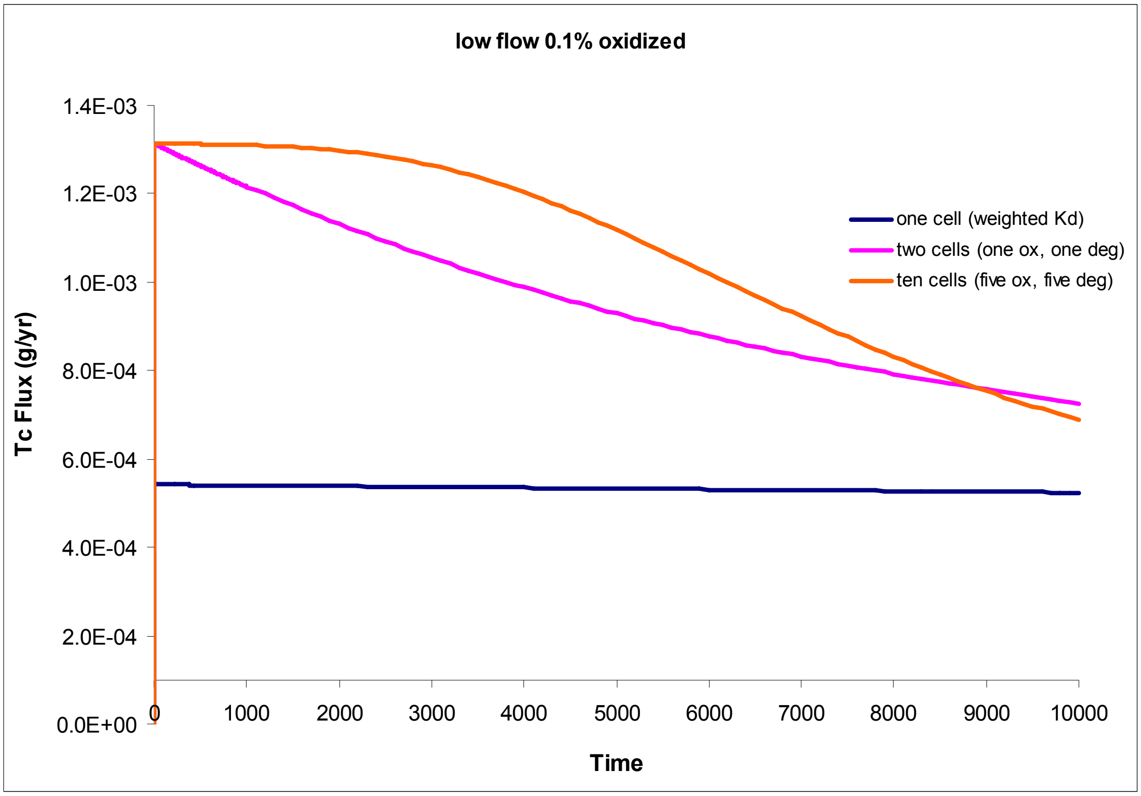


Figure 3: Modeled Tc flux from grout assuming 0.1% oxidized and low flow

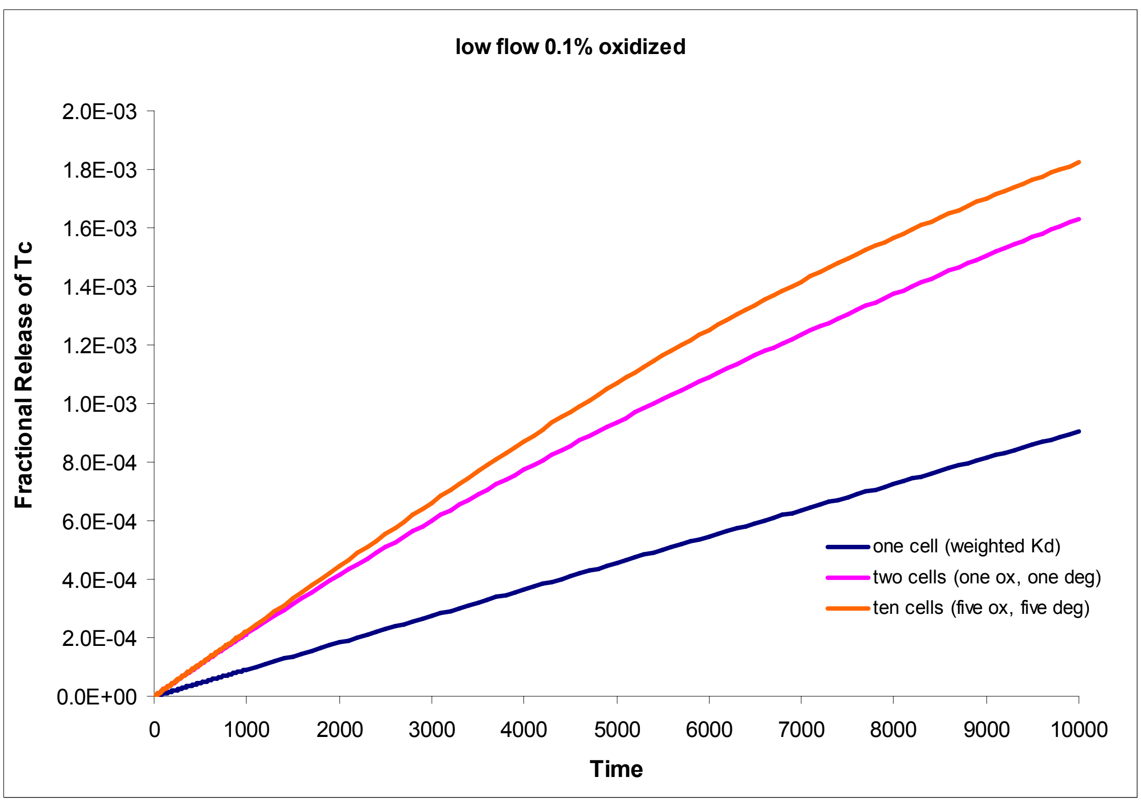
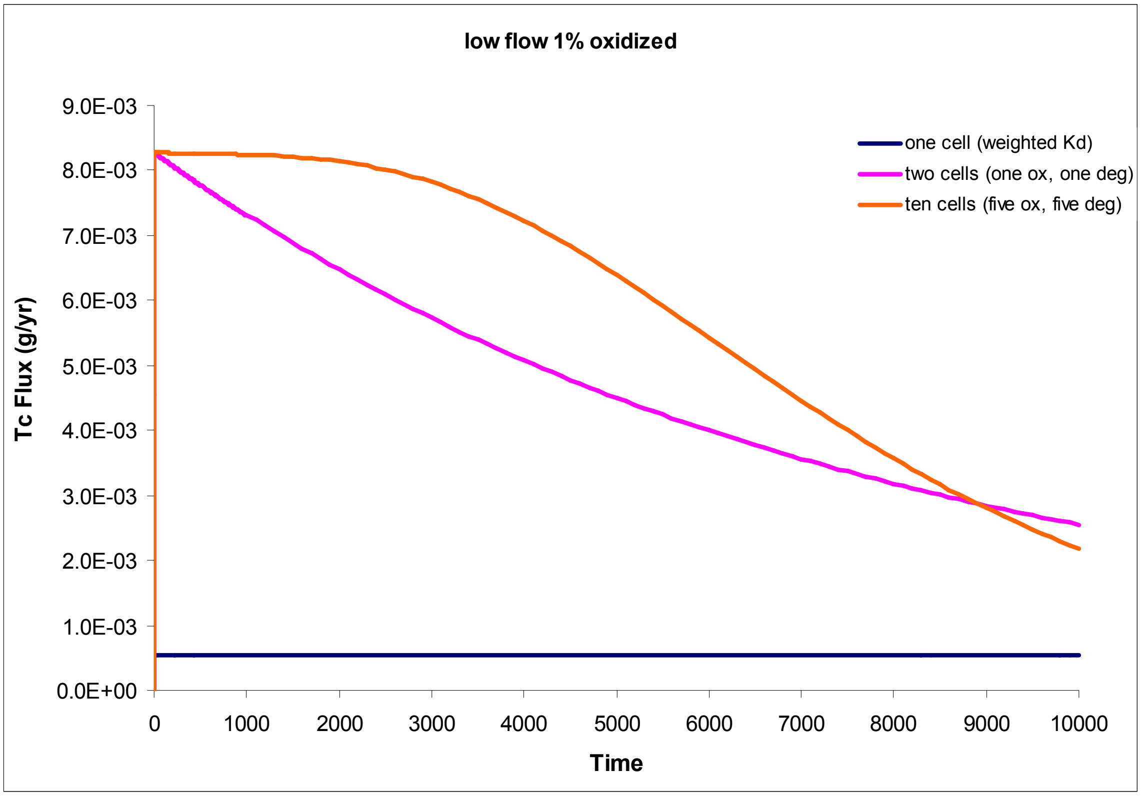


Figure 4: Cumulative fractional release of Tc assuming 0.1% oxidized and low flow



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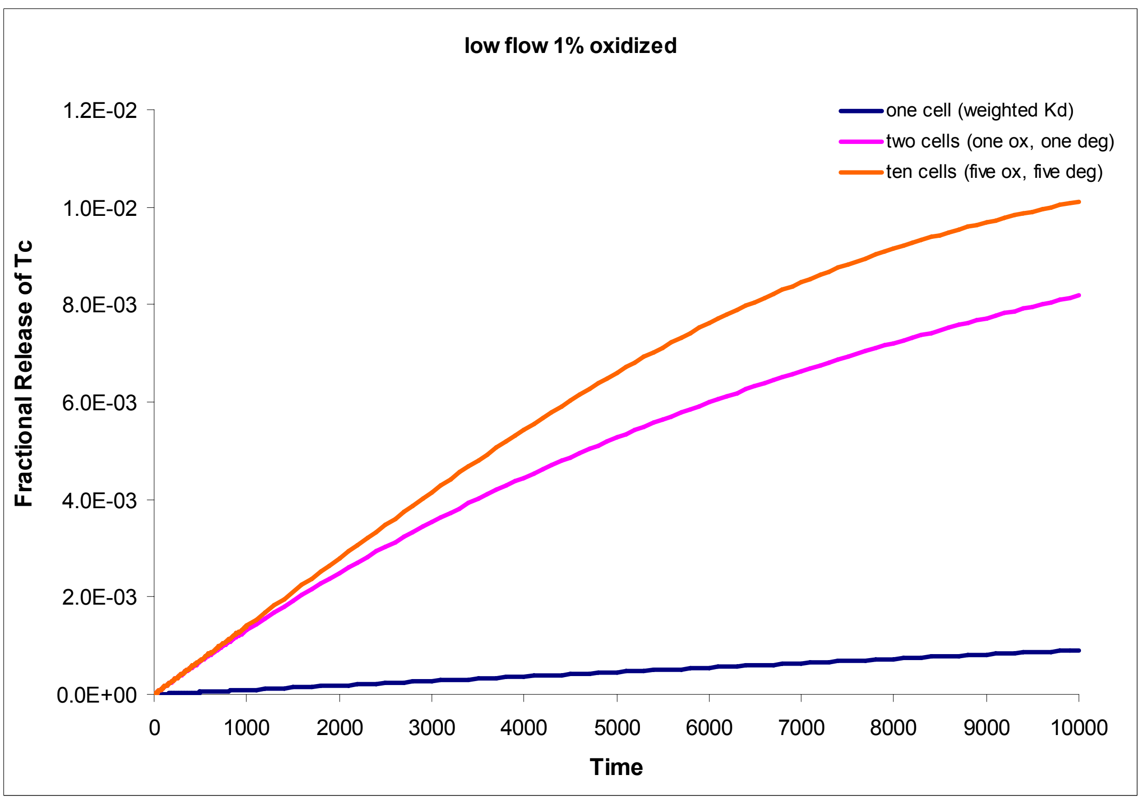
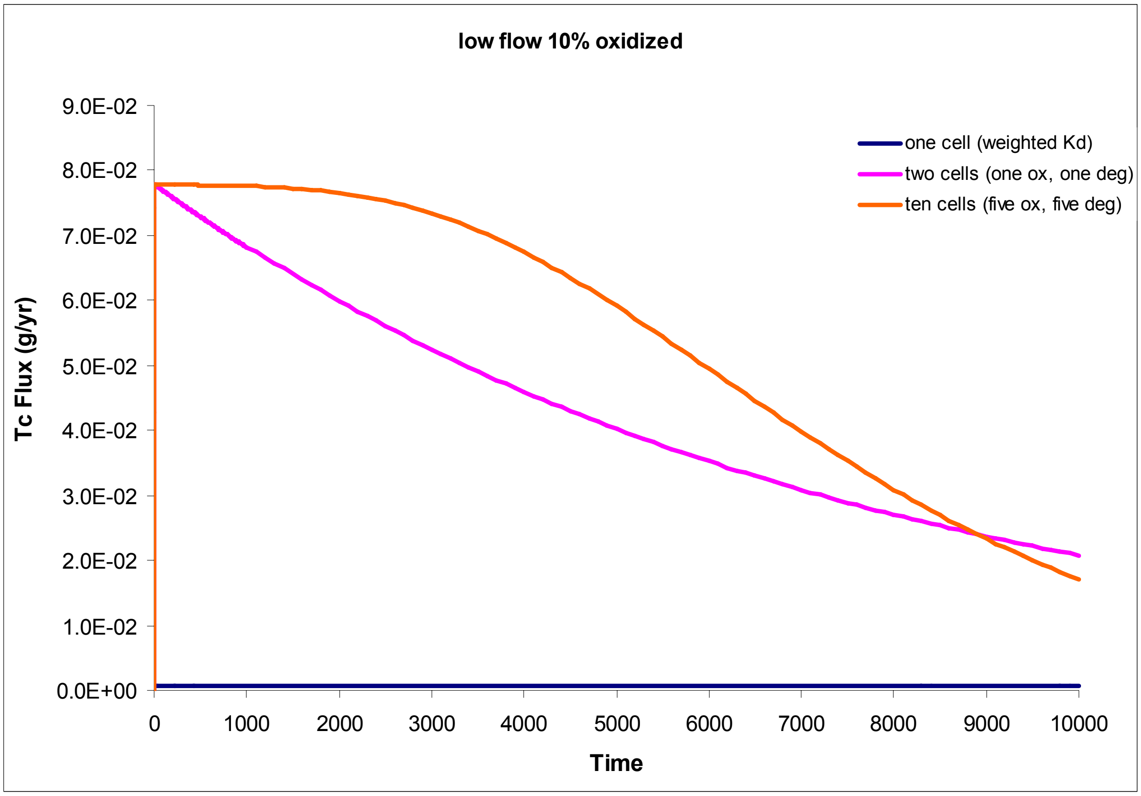


Figure 6: Cumulative fractional release of Tc assuming 1% oxidized and low flow



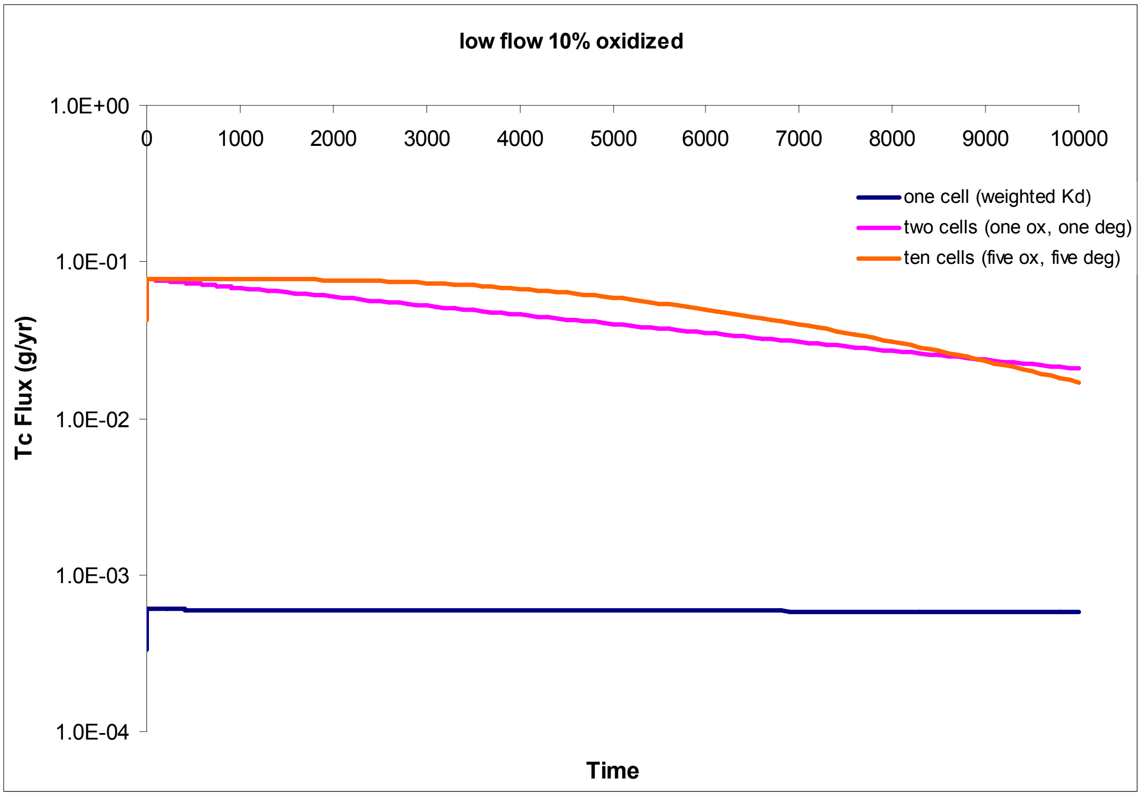


Figure 7: Modeled Tc flux from grout assuming 10% oxidized and low flow

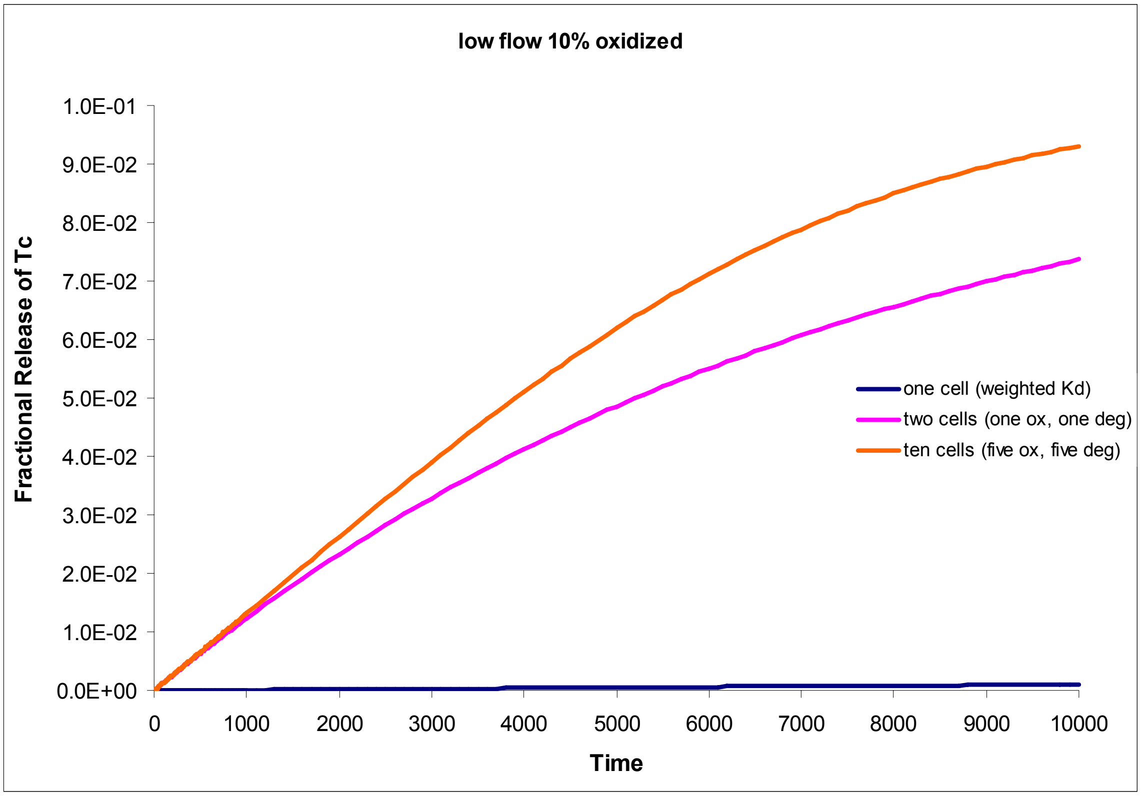


Figure 8: Cumulative fractional release of Tc assuming 10% oxidized and low flow

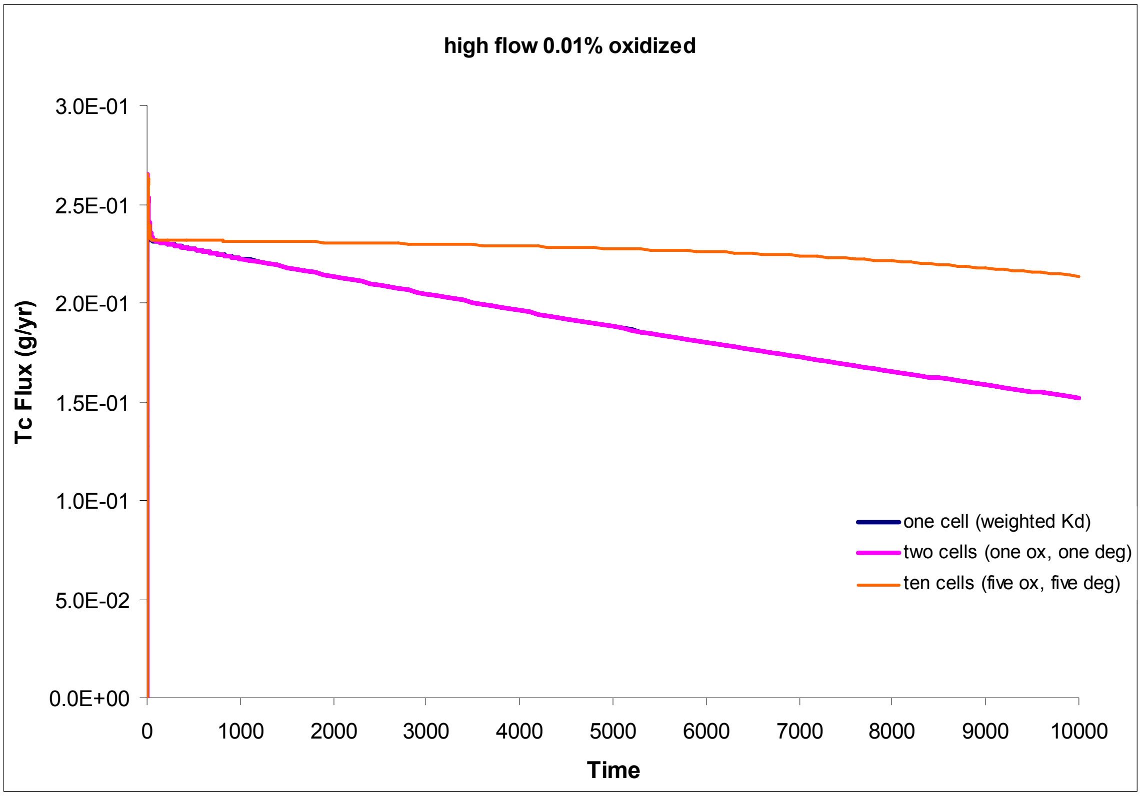


Figure 9: Modeled Tc flux from grout assuming 0.01% oxidized and high flow *

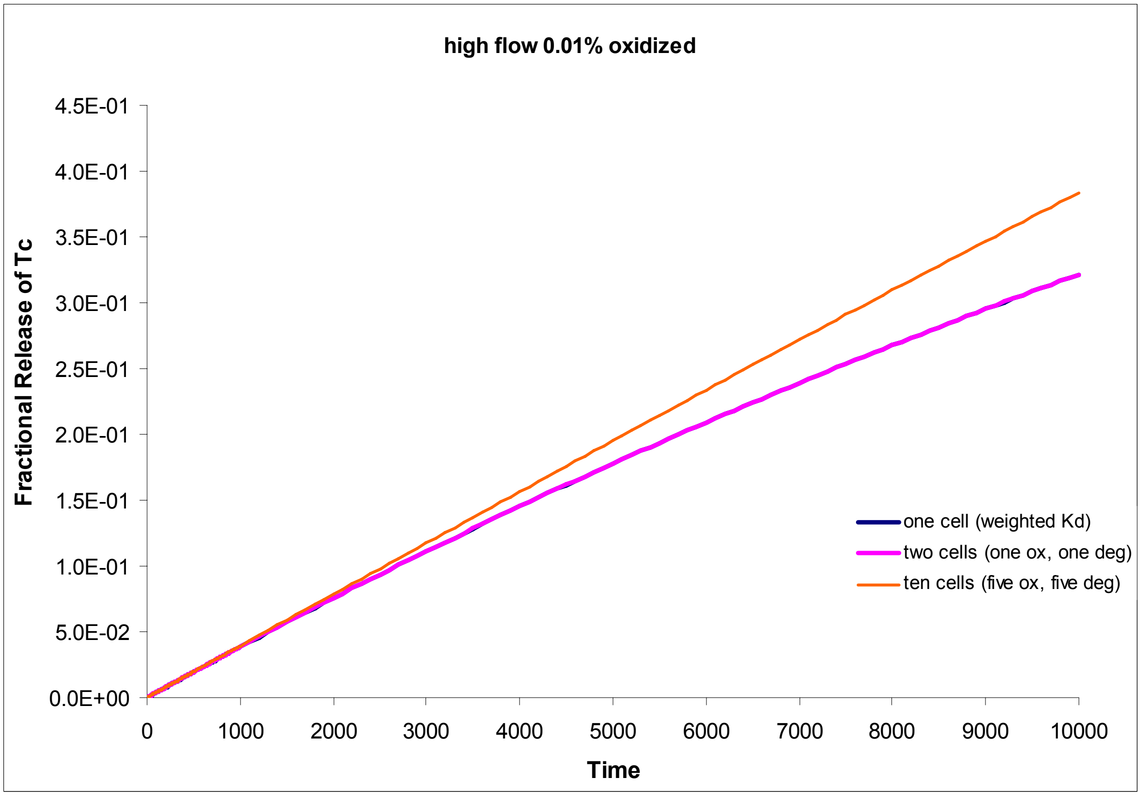
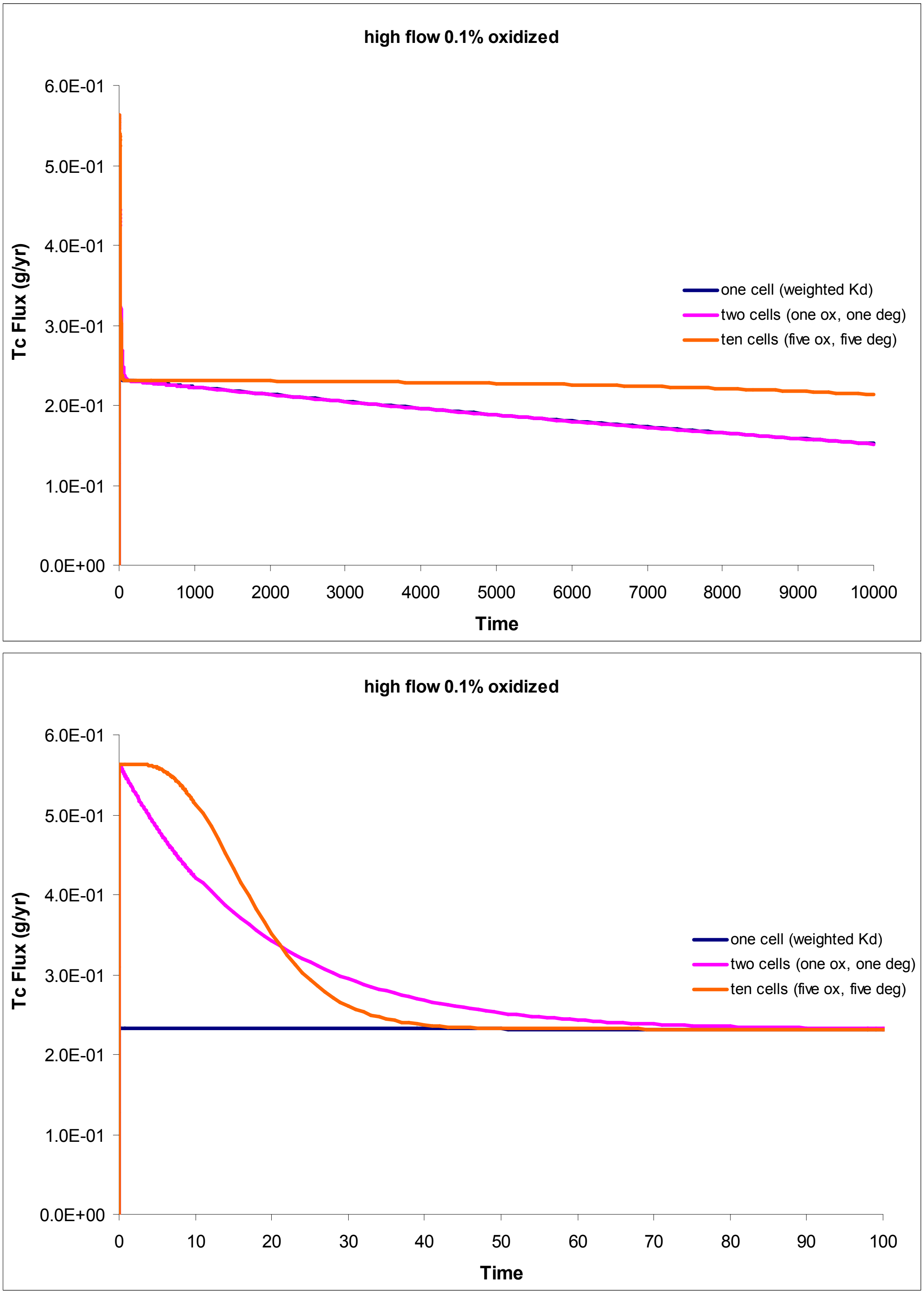


Figure 10: Cumulative fractional release of Tc assuming 0.01% oxidized and high flow *

** note that the one cell and two cell fluxes overlap*



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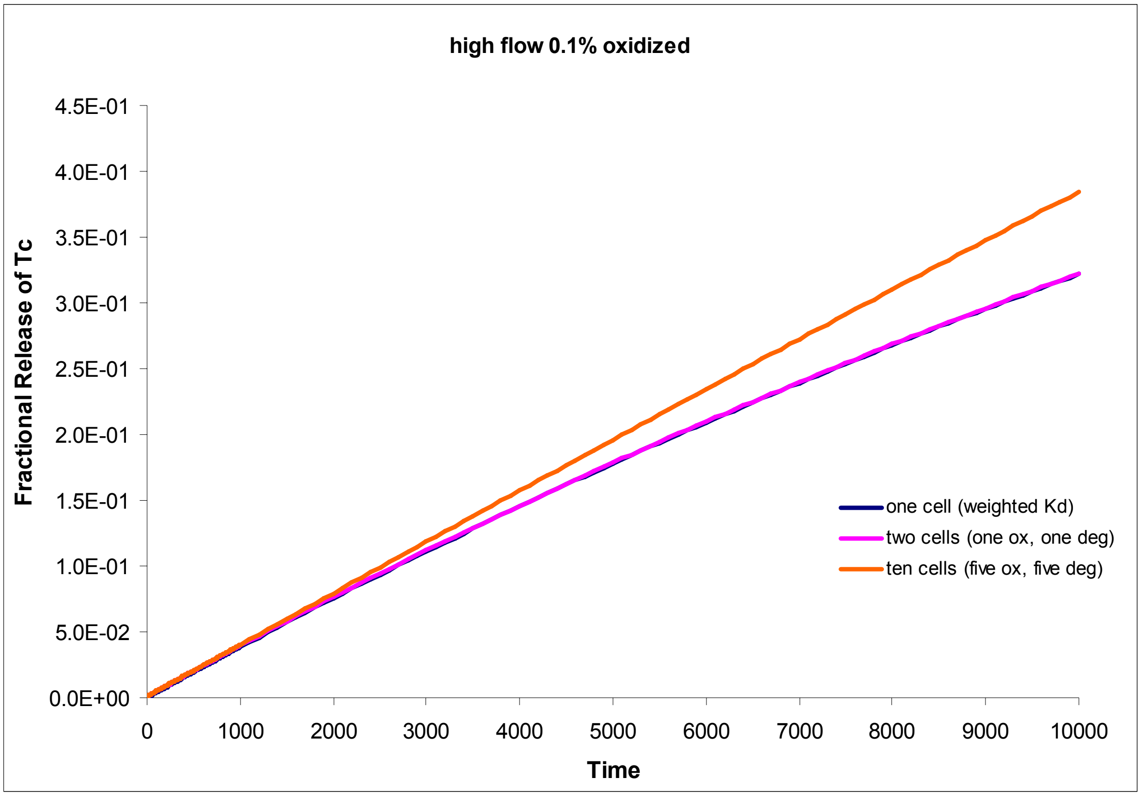
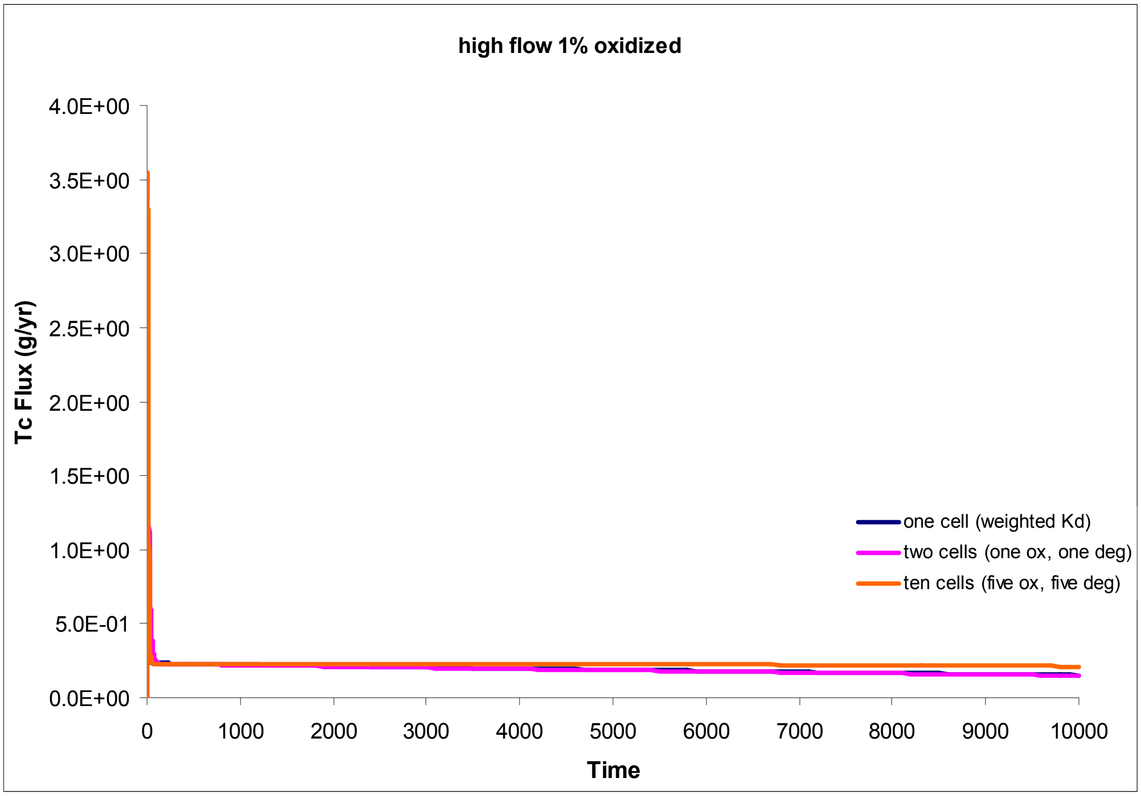


Figure 12: Cumulative fractional release of Tc assuming 0.1% oxidized and high flow

** note that the one cell and two cell fractional releases overlap*



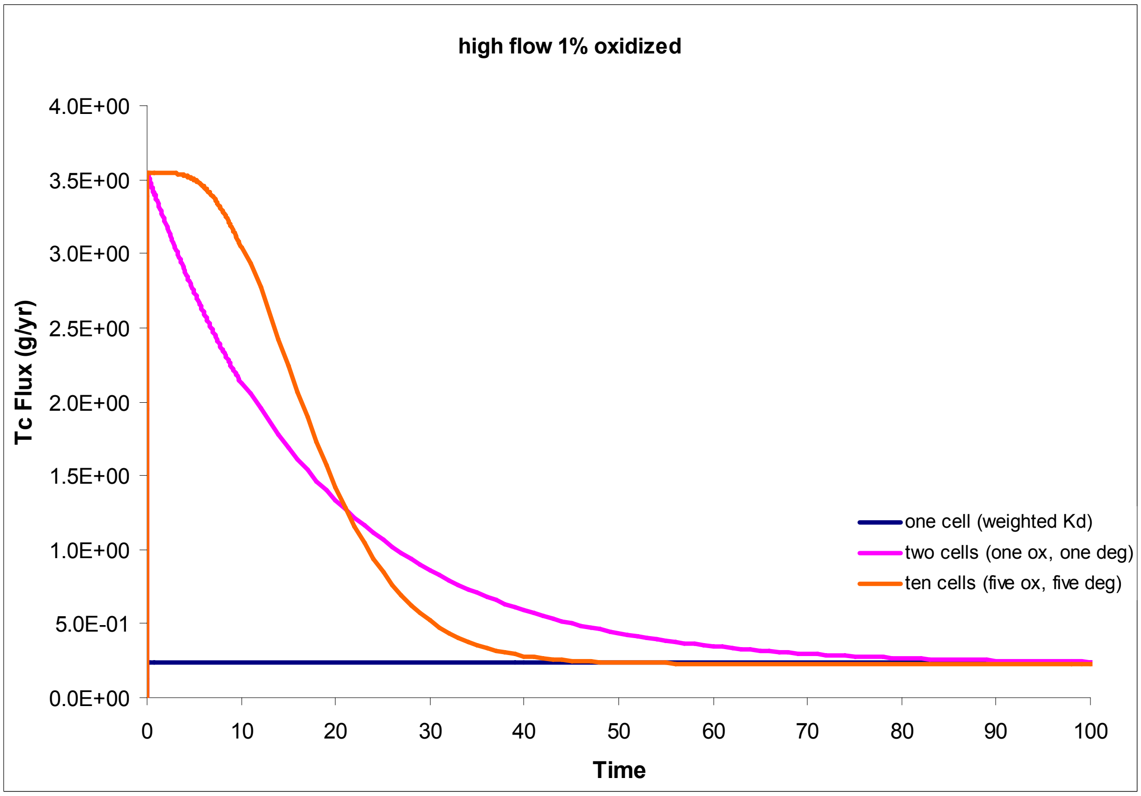
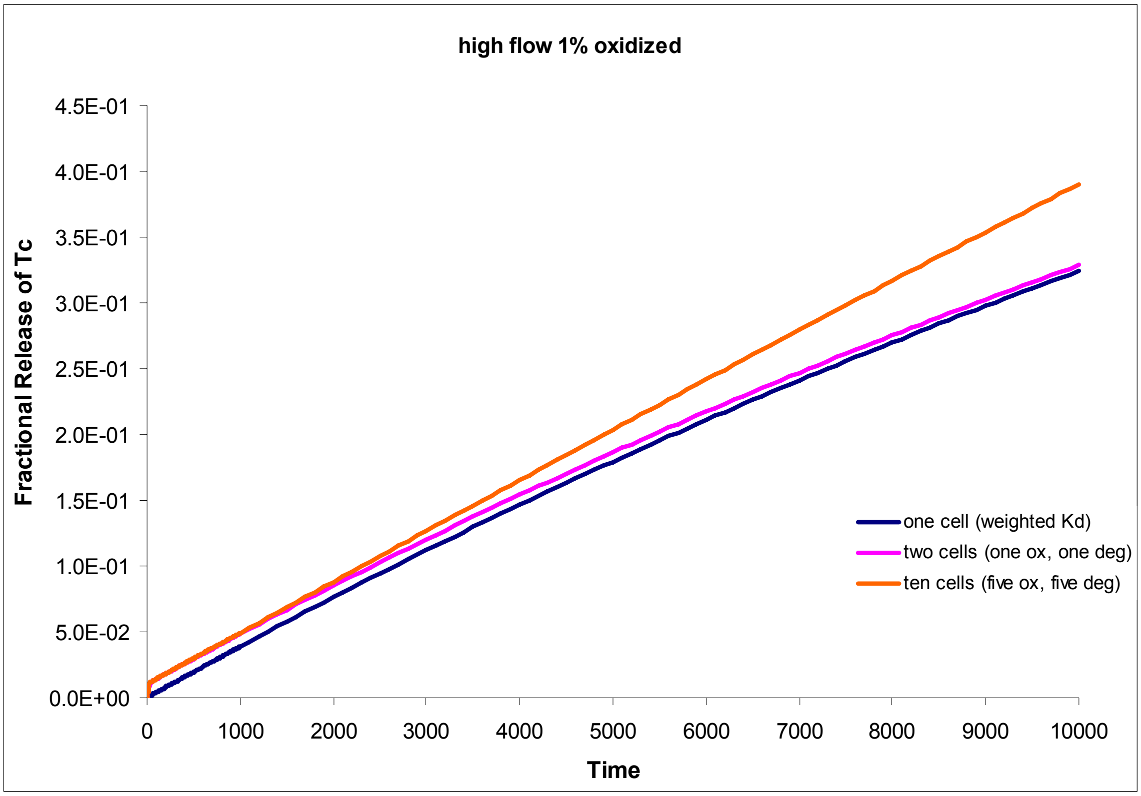


Figure 13: Modeled Tc flux from grout assuming 1% oxidized and high flow



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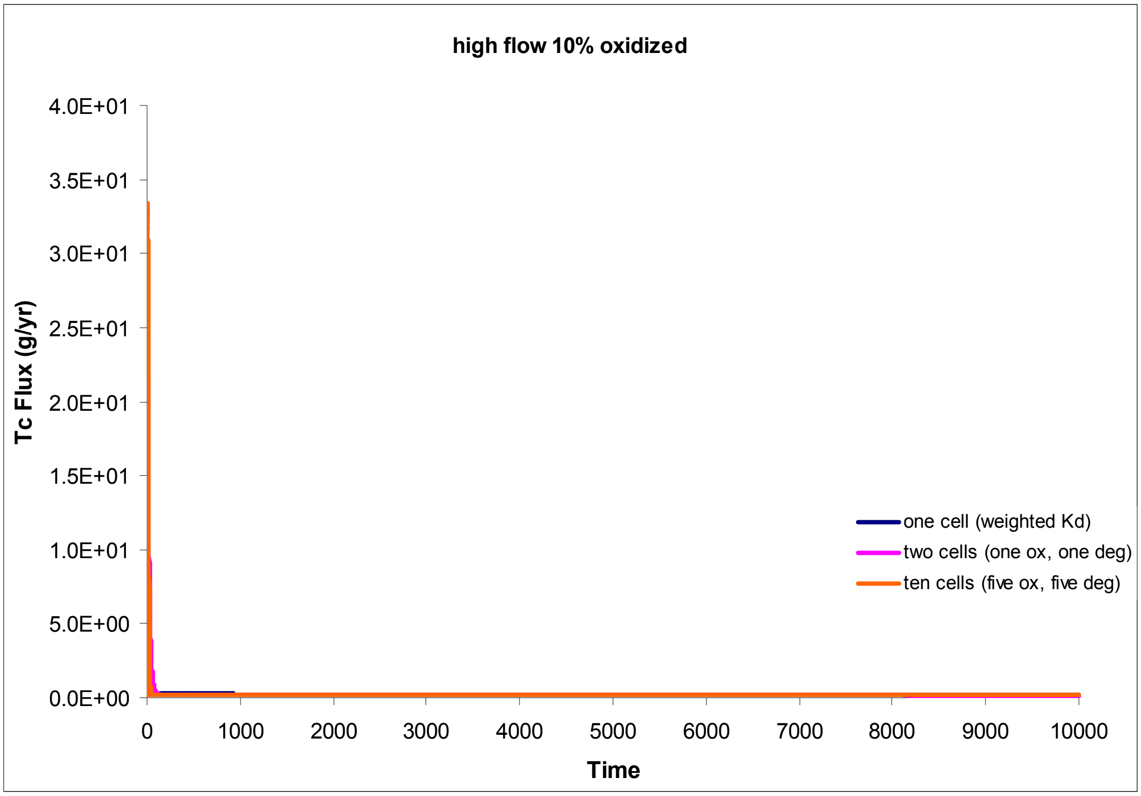


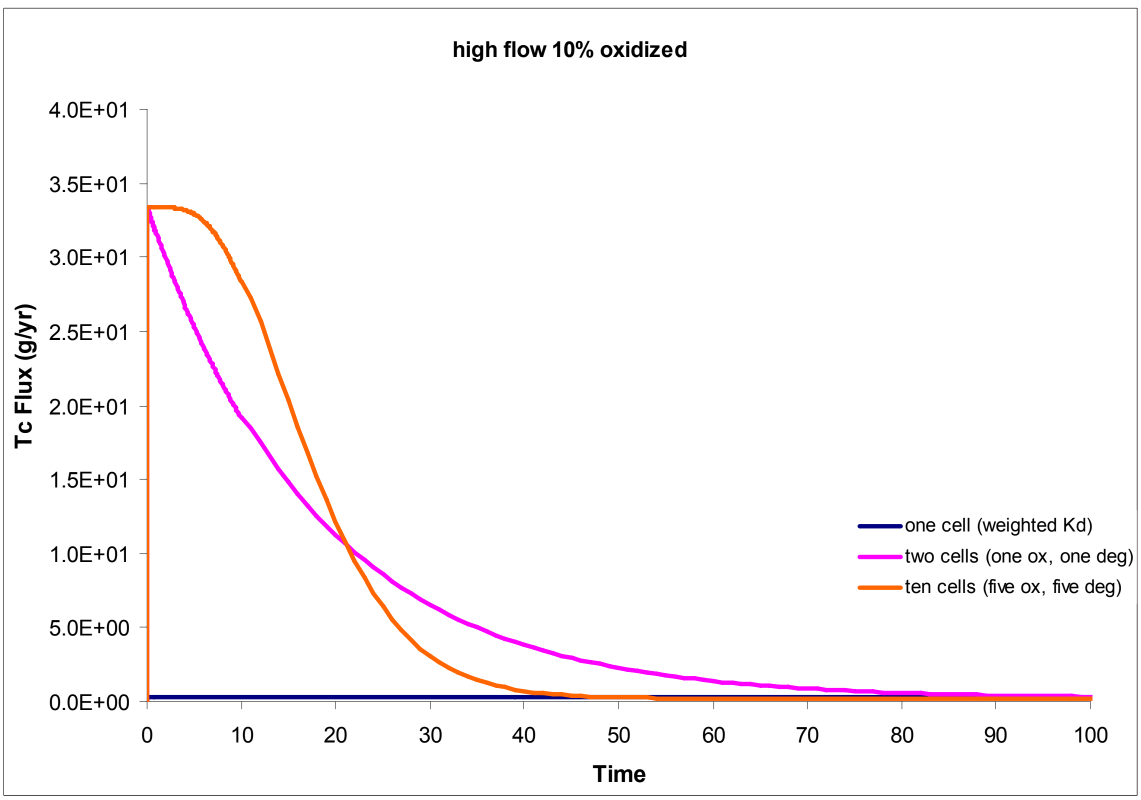
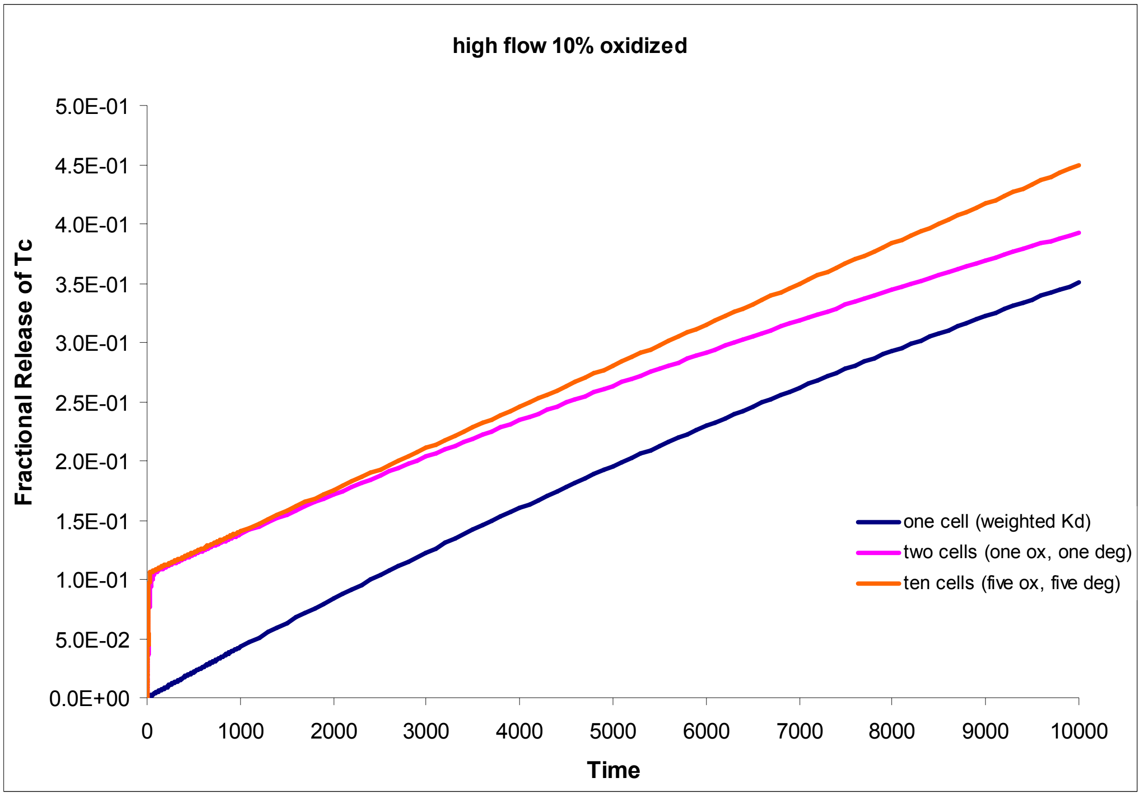


Figure 15: Modeled Tc flux from grout assuming 10% oxidized and high flow



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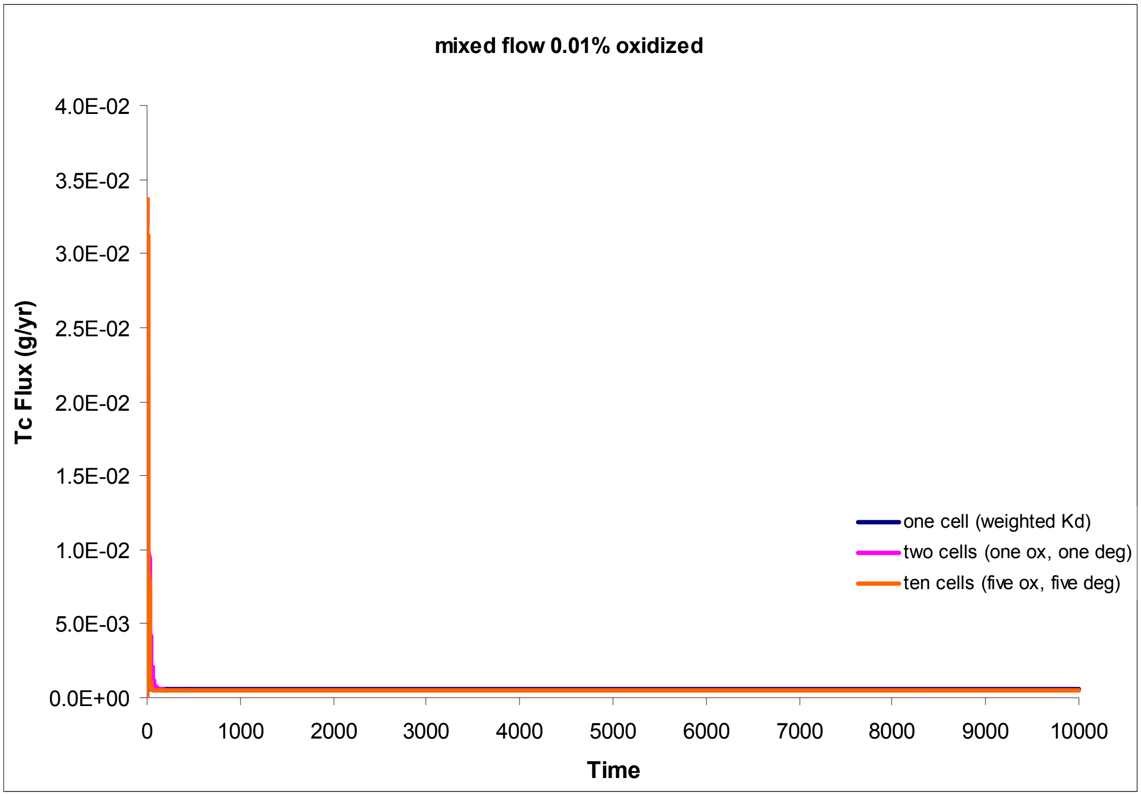


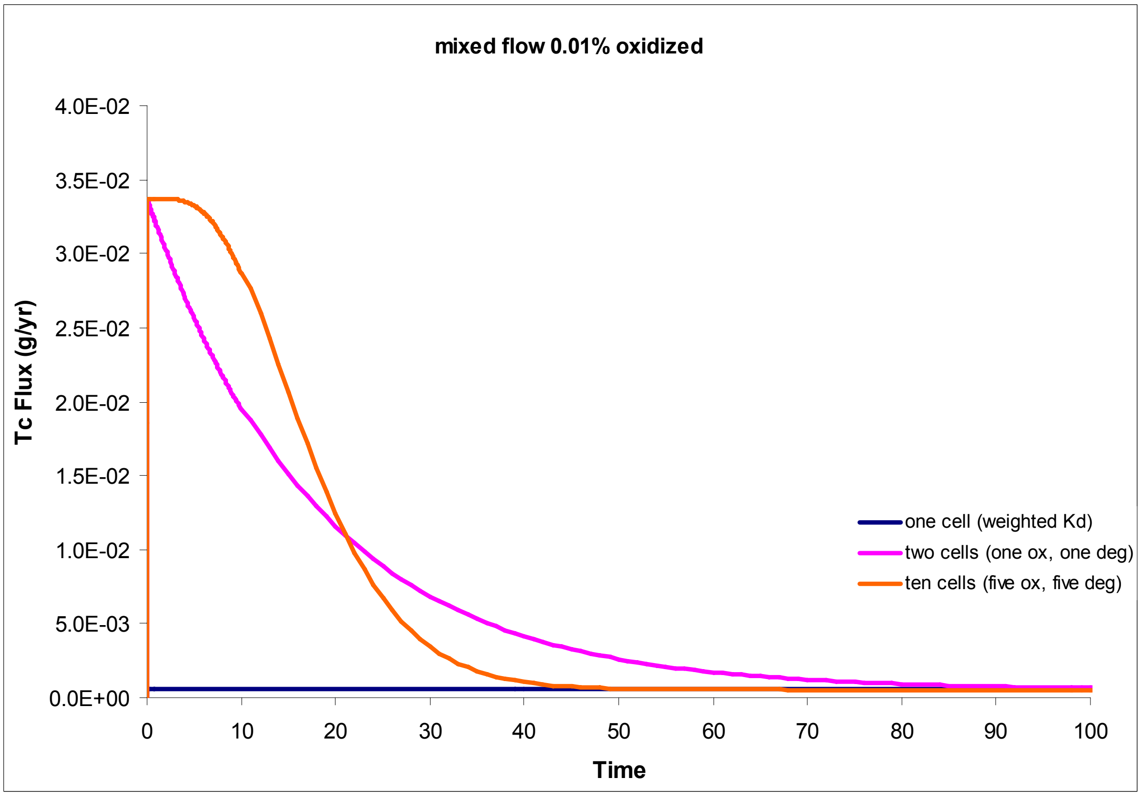


Figure 17: Modeled Tc flux from grout assuming 0.01% oxidized and mixed flow

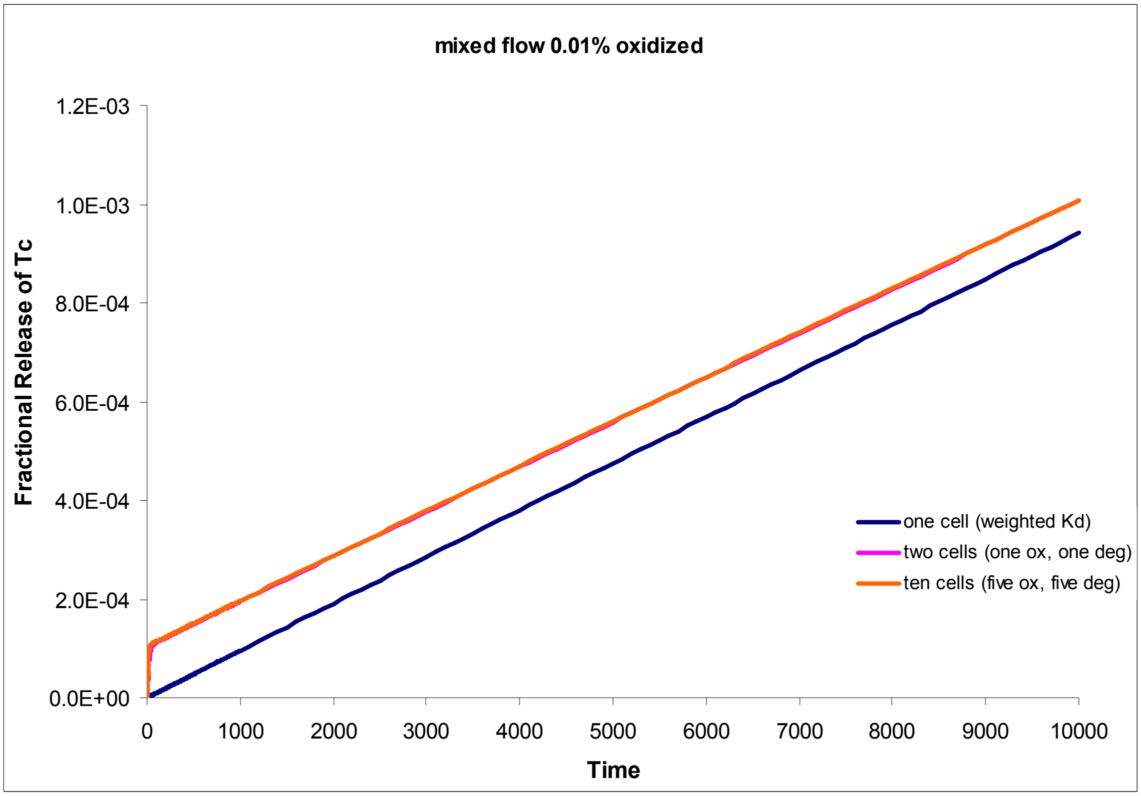


Figure 18: Cumulative fractional release of Tc assuming 0.01% oxidized and mixed flow

** note that the two cell and ten cell fractional releases overlap*

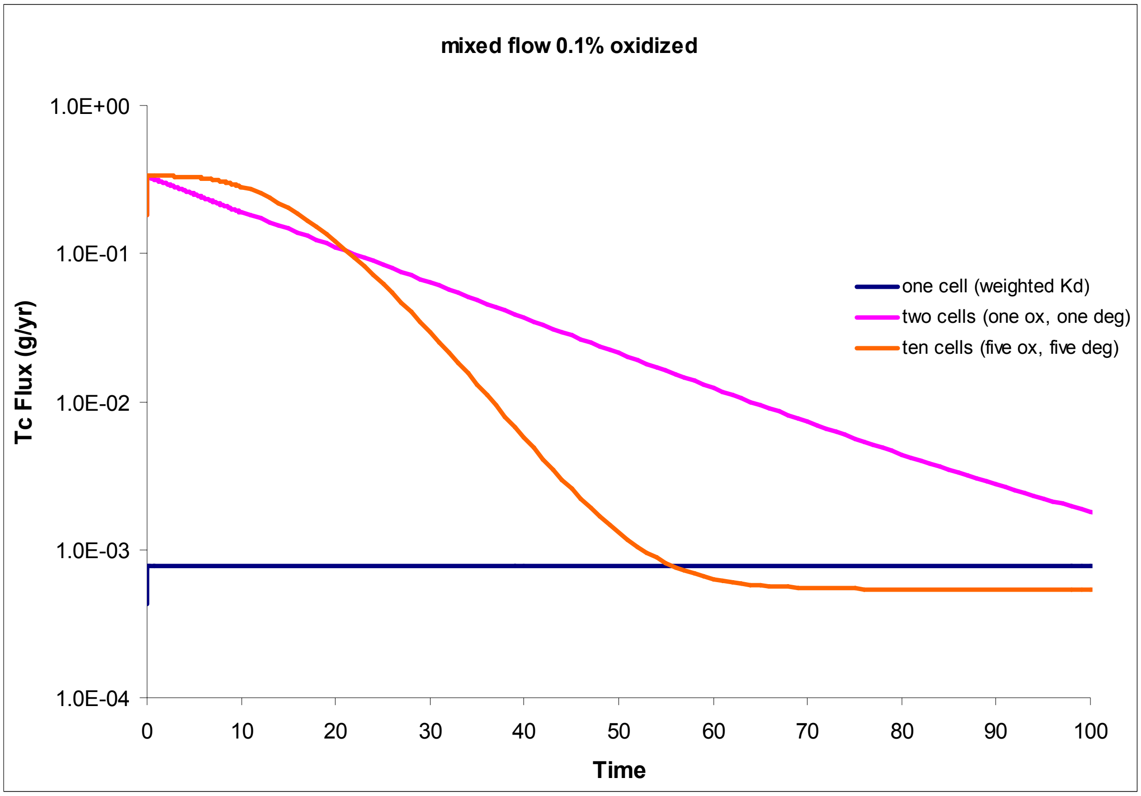


Figure 19: Modeled Tc flux from grout assuming 0.1% oxidized and mixed flow

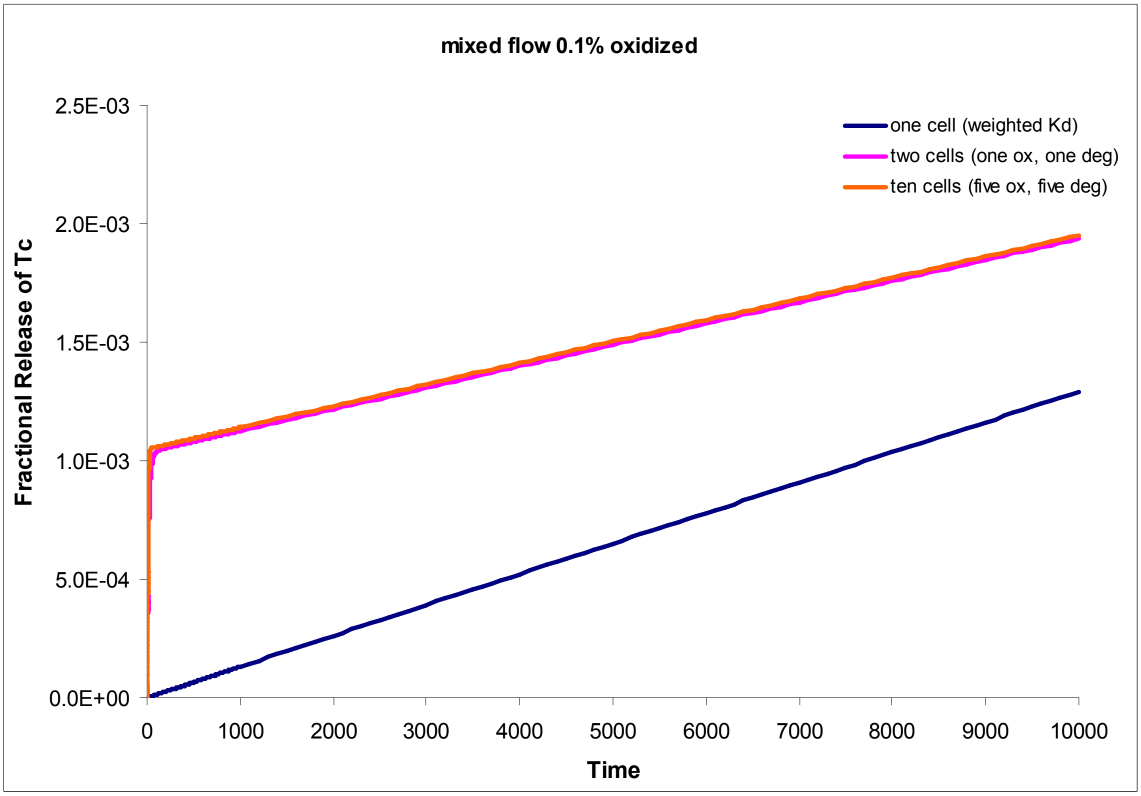
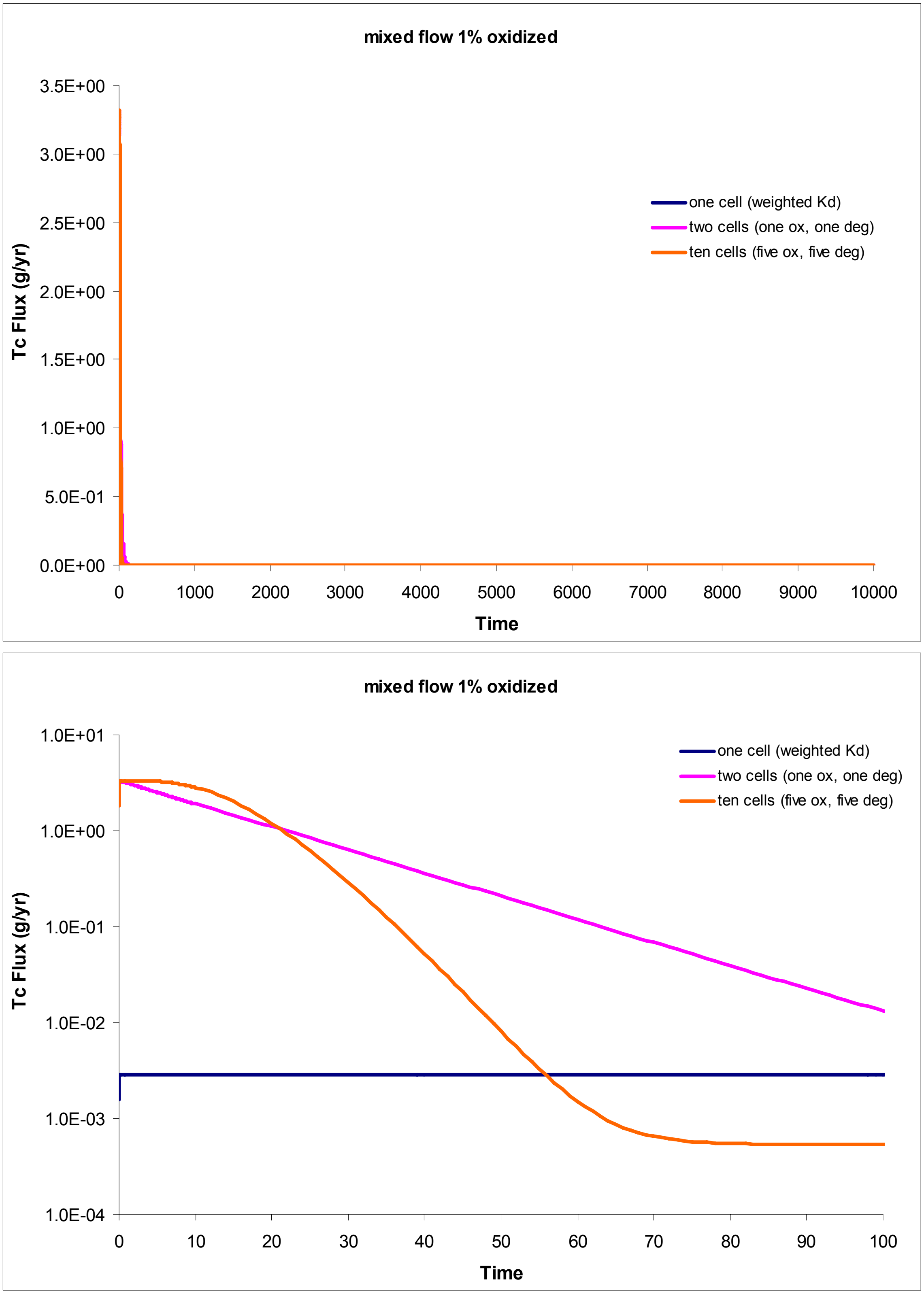


Figure 20: Cumulative fractional release of Tc assuming 0.1% oxidized and mixed flow
*** note that the two cell and *ten cell* fractional releases overlap**



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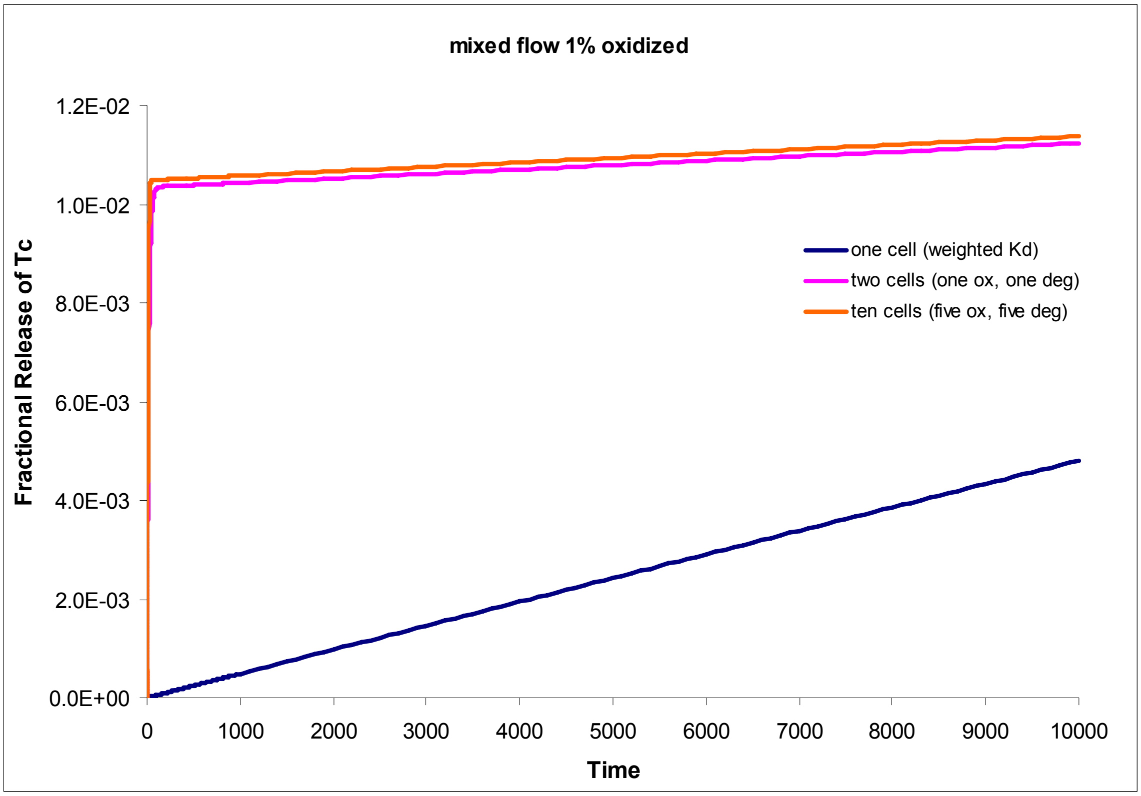
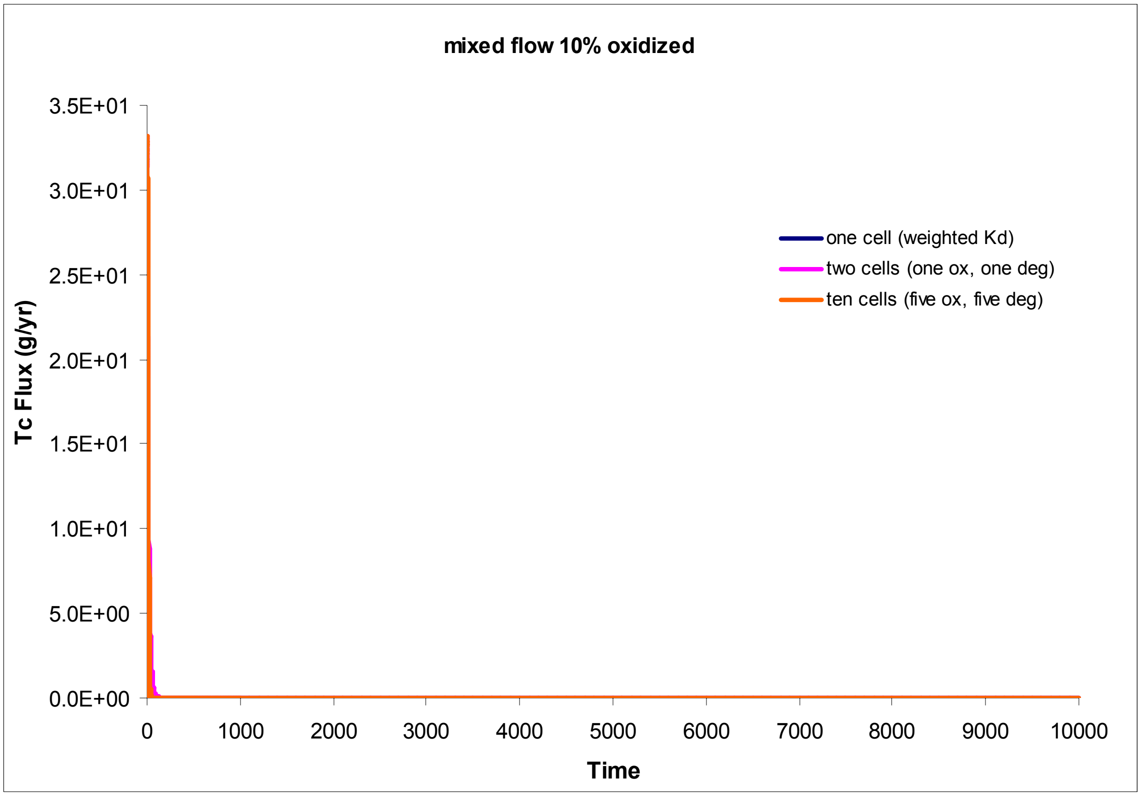


Figure 22: Cumulative fractional release of Tc assuming 1% oxidized and mixed flow



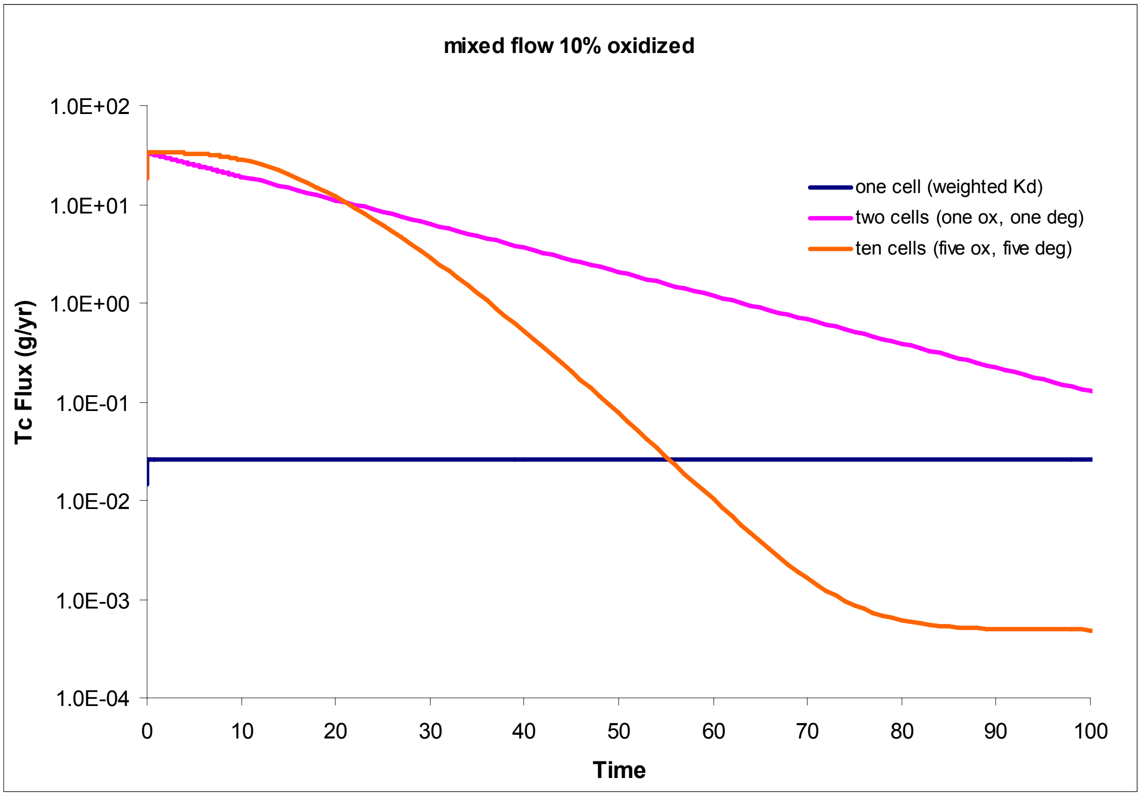
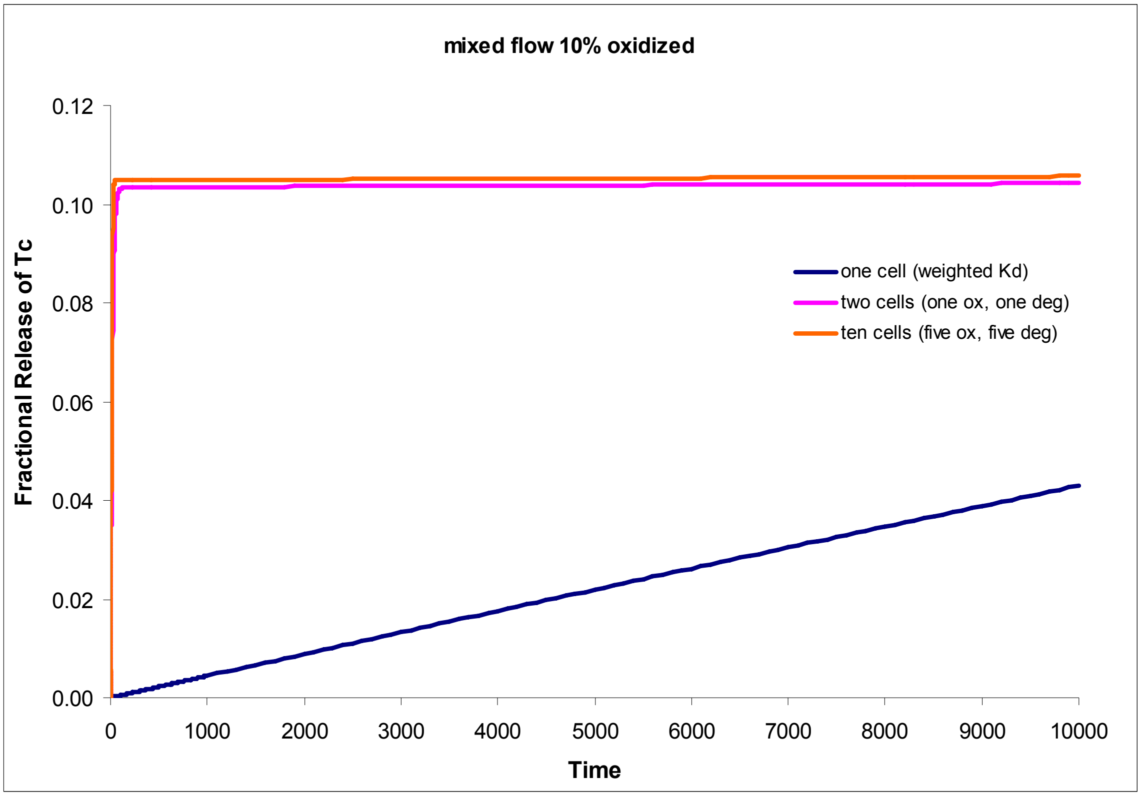


Figure 23 : Modeled Tc flux from grout assuming 10% oxidized and mixed flow



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