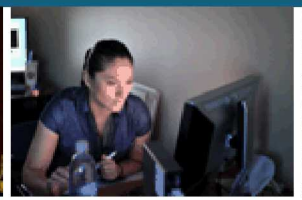
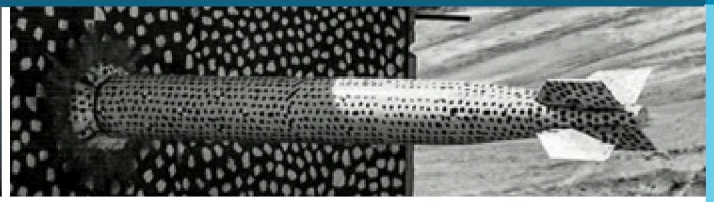
SAND2019-5511C

Benchmarking and QA Testing PFLOTRAN





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Motivation

An important early step in QA is to verify a code against analytical solutions

Analytical solutions are typically too simple to be representative of realistic scenarios, however if each part of the equations has been demonstrated to provide the correct solution, confidence is gained that the full set of equations are implemented correctly and accurately

In this work a series of PFLOTRAN QA tests are conducted for one-dimensional, transient equations in two-phase flow that have known analytical solutions

This work:

- Tests numerical implementation of relations in the code and demonstrates the accuracy of the simulated solution for a simplified set of equations and geometries
- Rigorously demonstrates convergence of PFLOTRAN to analytical solutions

Equations with analytical solutions for two-phase flow

Fluid flow

$$\varphi \frac{\partial C_i}{\partial t} + v \frac{\partial F_i}{\partial x} = 0$$

Temperature

$$\frac{\partial T}{\partial t} + g \frac{\partial T}{\partial x} = 0$$

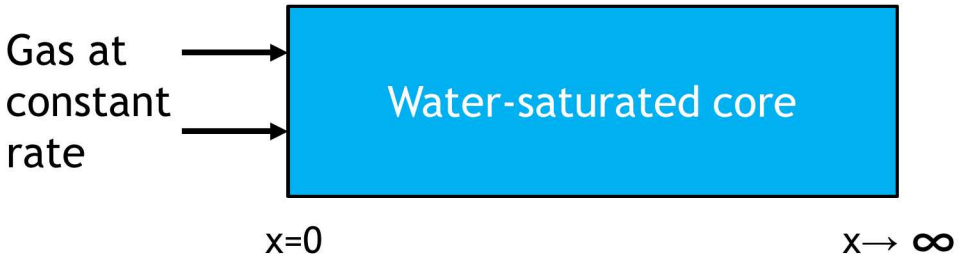
where $C_i = \sum_{j=1}^{2} c_{ij} \rho_j S_j$ $F_i = \sum_{j=1}^{2} c_{ij} \rho_j f_j$

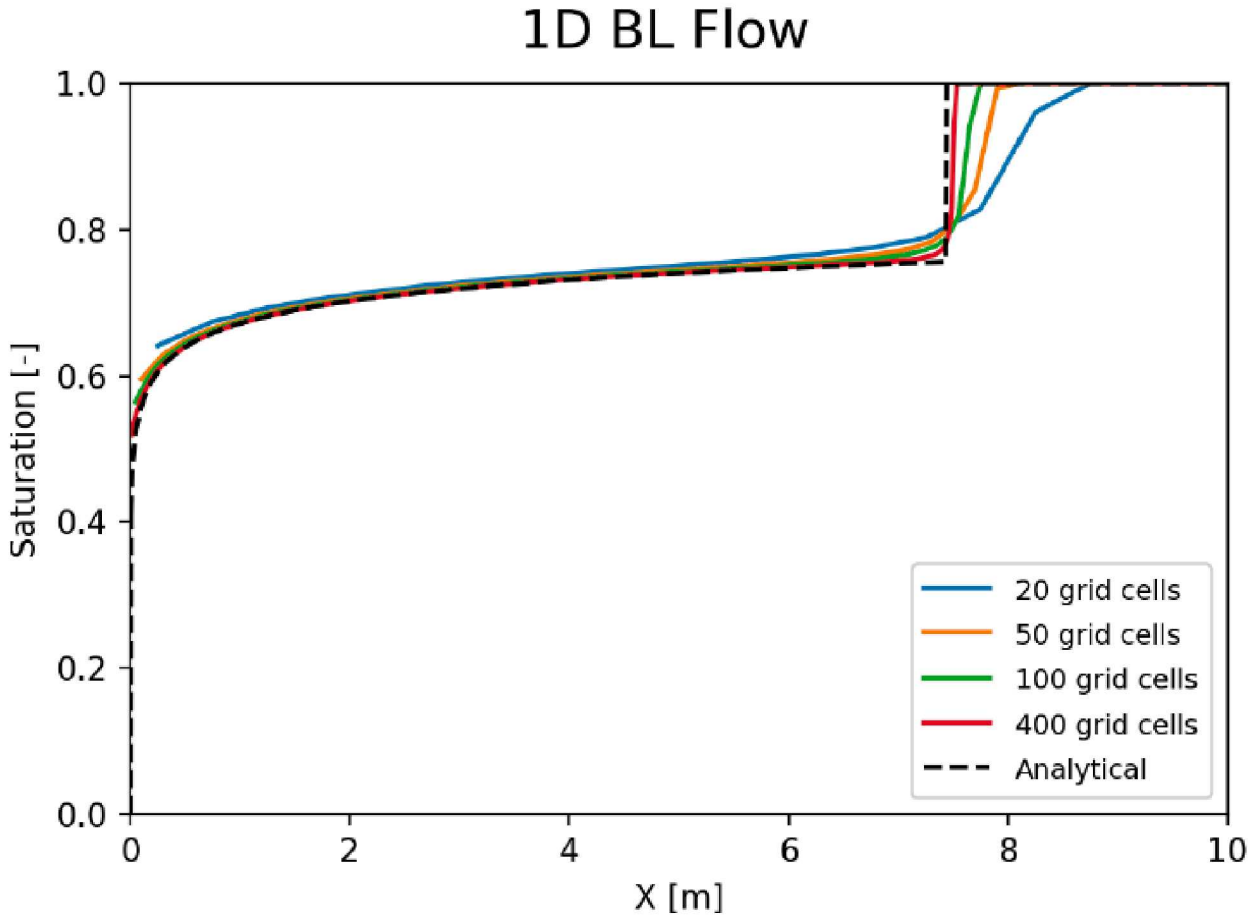
and flux terms f_j and g are $f_j = \frac{k_{rj}/\mu_j}{k_{r1}/\mu_1 + k_{r2}/\mu_2}$ $g = \frac{f_1 + \alpha}{S_1 + \beta}$

Error metrics: $L2 = \frac{\sqrt{\Sigma (Q^{sim} - Q^{an})^2}}{\sqrt{\Sigma (Q^{an})^2}}$ $L1 = \frac{\Sigma |Q^{sim} - Q^{an}|}{\Sigma |Q^{an}|}$

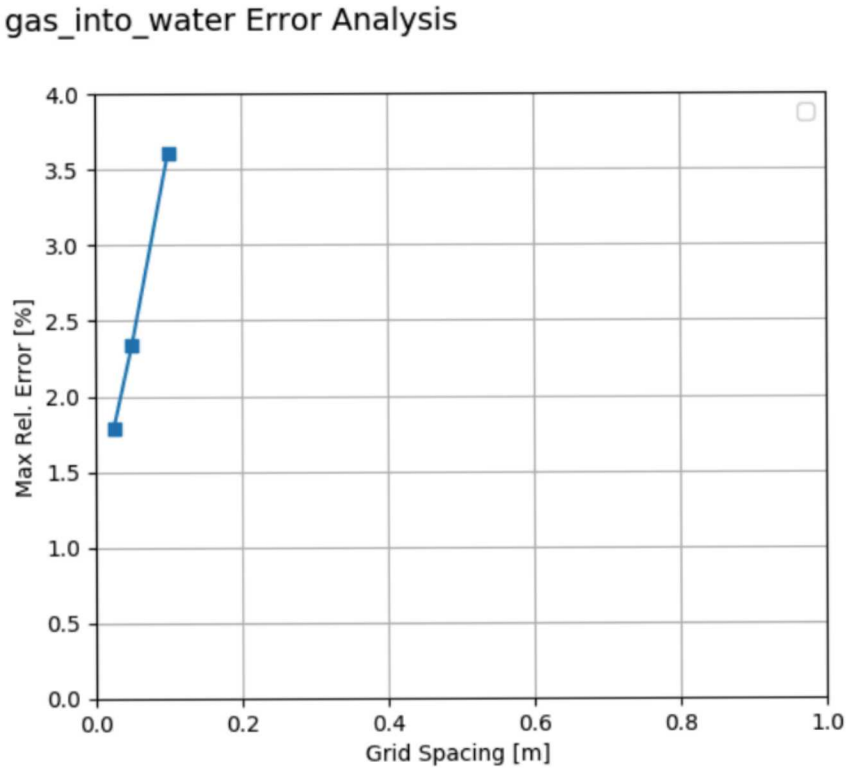
Model 1: Immiscible, isothermal linear flow (Air injection)

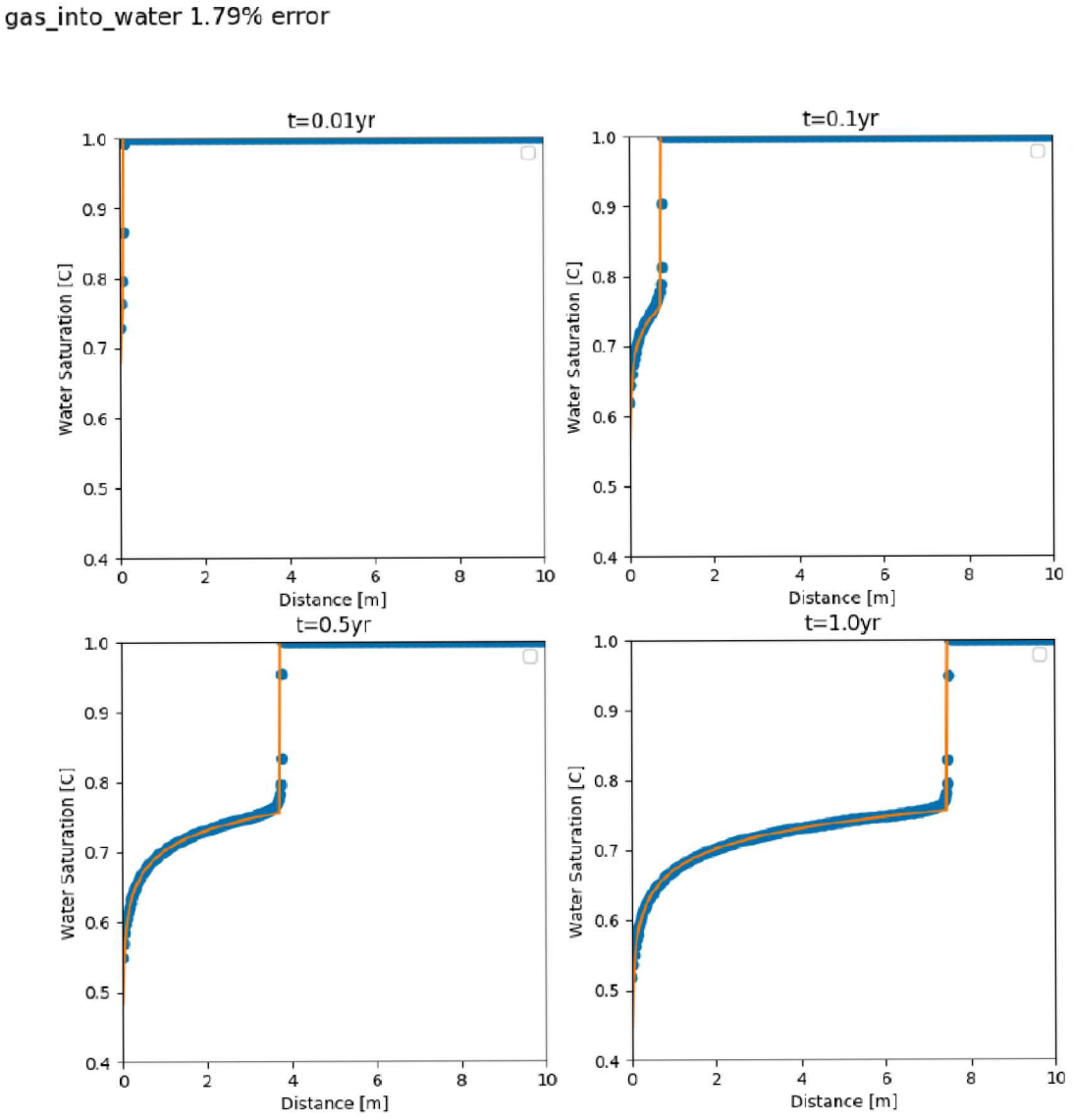
Schematic of Riemann problem



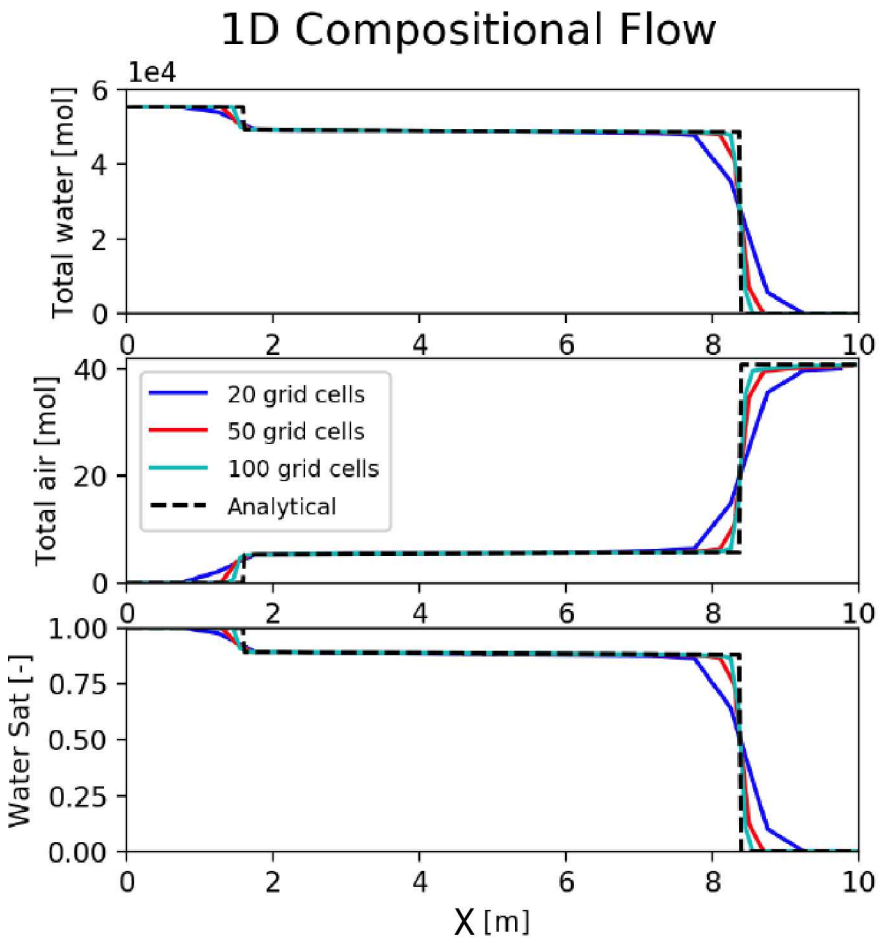


Model 1: QA test harness output (https://qa.pflotran.org)

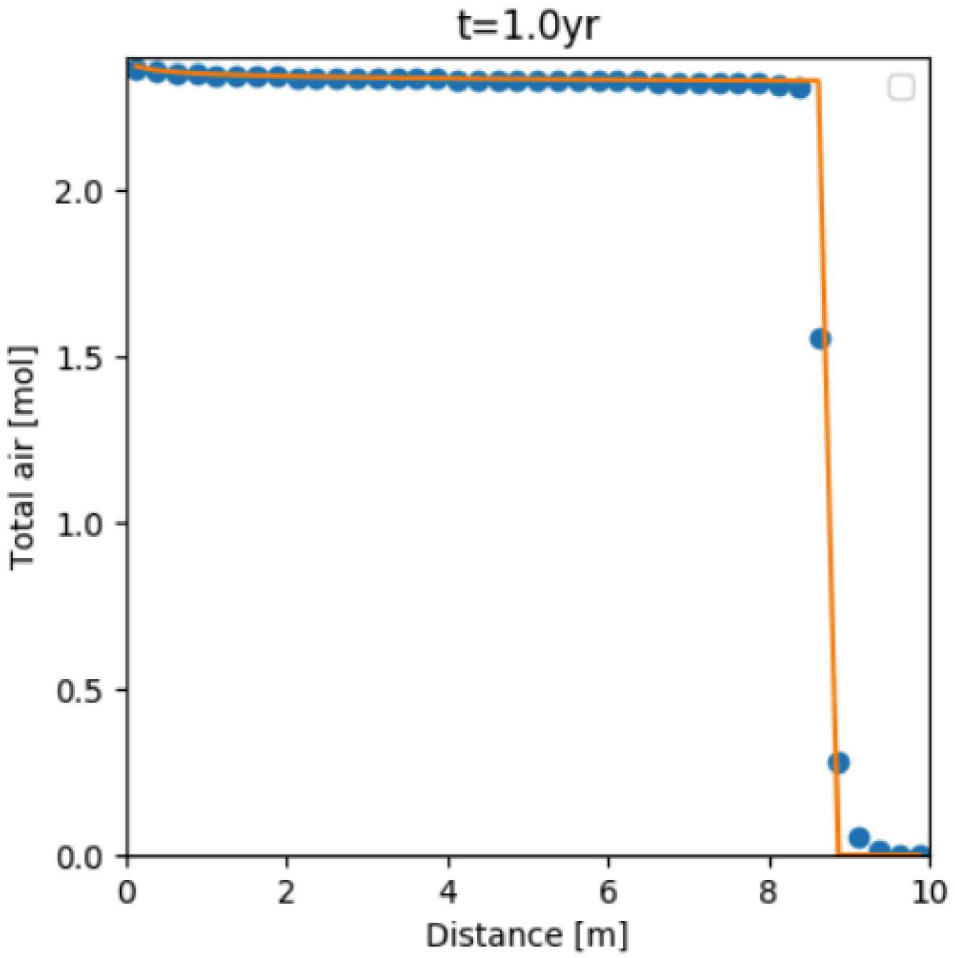




Model III and IV: Compositional, isothermal flow

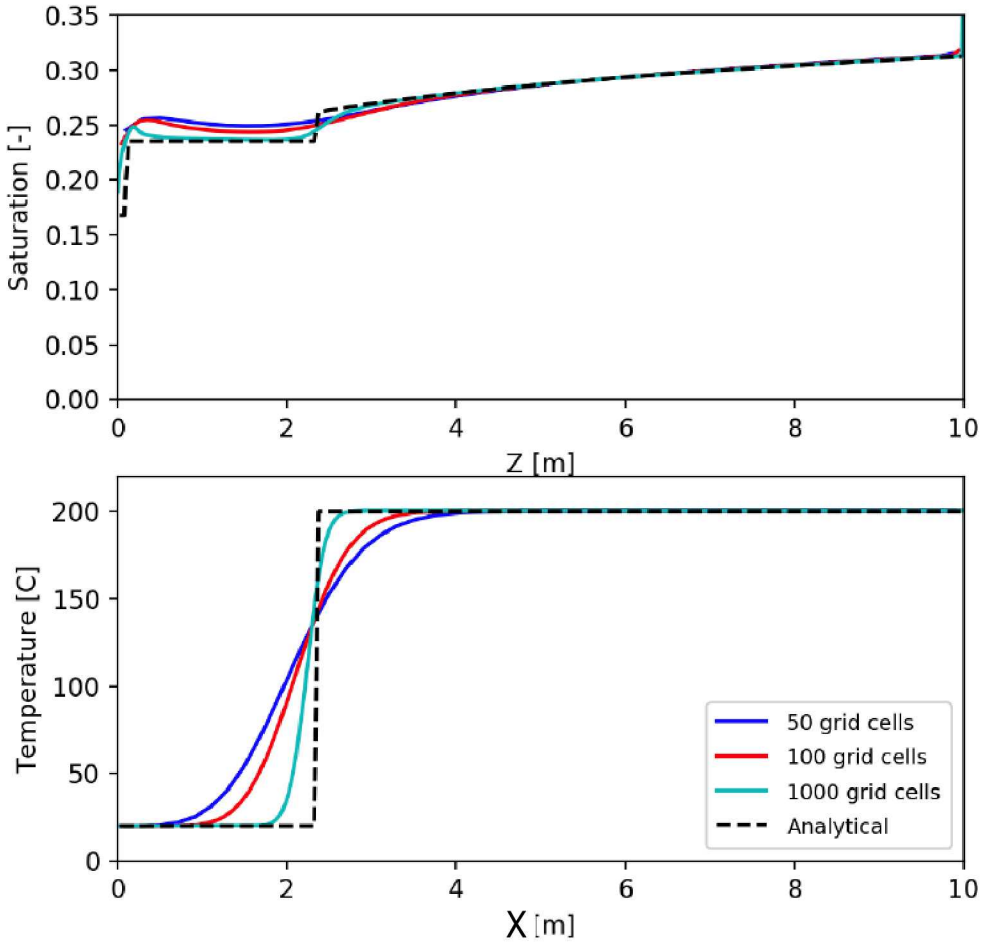


Model III: water injection into dry medium



Model IV: air injection into saturated medium

Model VIII: Immiscible, non-isothermal flow



Model VIII: cold air injection into saturated medium

Results summary

Name	Model details	Grid cells to convergence (norm used)	Time to convergence
Model 1	Injection of air into a completely saturated linear aquifer with immiscible fluids.	400 (L2)	44 sec
Model 2	Air injection into a radial aquifer with properties identical to Model 1.	100 (L2)	3.0 sec
Model 3	Water injection into a completely dry linear porous media with component partitioning.	100 (L1)	5.4 min
Model 4	Air injection into a completely saturated linear aquifer with component partitioning.	40 (L1)	18 sec
Model 5	Water injection into a completely dry radial porous media with identical flow properties as Model 3	80 (L1)	3.2 min
Model 6	Air injection into a completely saturated aquifer with identical flow properties as Model 4	80 (L1)	23 sec
Model 7	CO_2 injection into a completely saturated linear aquifer.	480 (L1)	6.8 min
Model 8	Injection of cold air into a completely saturated linear aquifer.	1000 (L1)	4.2 min

Conclusions

PFLOTRAN has been shown to converge to the exact analytical solution for eight very stiff two-phase, transient flow problems

In each case PFLOTRAN converges to within 2% of the analytical solution based on a rigorous error metric

This demonstrates that the implementation of the equations for these models are correct and that the approximation in the numerical method is accurate with sufficient grid resolution

Time it takes for solutions to converge depends on both physics of the model and boundary conditions

All convergence tests are available in the PFLOTRAN QA test harness at https://qa.pflotran.org

Thank you for listening