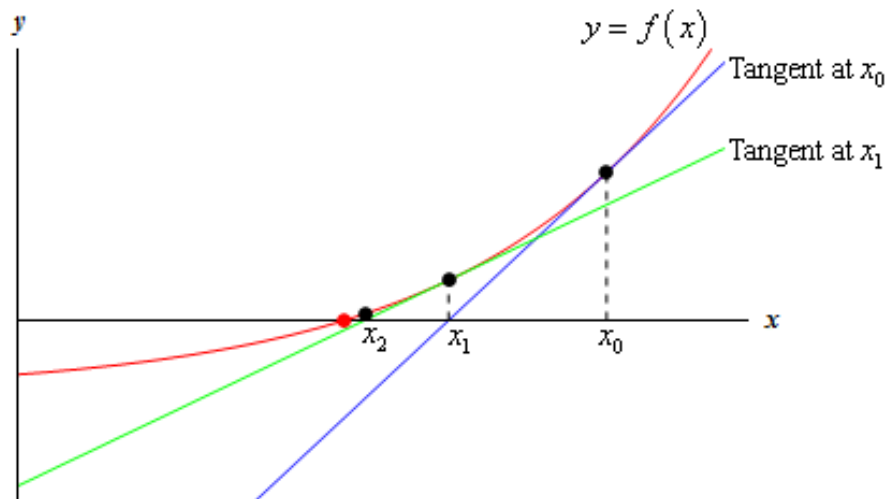


## Implementation of Analytical Derivatives within PFLOTRAN

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**SFWST LV Meeting**  
**May 24, 2017**



$$f(x_0) + f'(x_0)(x_1 - x_0) = 0$$

$$x_1 = x_0 - \frac{f(x_0)}{f'(x_0)}$$

$$f(x) = x^2$$

$$f'(x)_{\text{analytical}} = 2x$$

$$f'(x)_{\text{numerical}} = \frac{f(x + \Delta x) - f(x)}{\Delta x}$$

$$f'(x)_{\text{numerical}} = \frac{(x + \Delta x)^2 - x^2}{\Delta x}$$

## Derivatives: Analytical vs. Numerical

---

$$x = 0.5$$

$$f(x) = x^2 = 0.5^2 = 0.25$$

$$f'(x)_{\text{analytical}} = 2x = 2 \cdot 0.5 = 1$$

$$\Delta x = 0.25$$

$$f'(x)_{\text{numerical}} = \frac{f(x + \Delta x) - f(x)}{\Delta x} = \frac{(x + \Delta x)^2 - x^2}{\Delta x} = \frac{(0.5 + 0.25)^2 - 0.5^2}{0.25} = 1.25$$

$x$	$f(x)$	$\Delta x$	$f(x + \Delta x)$	$f'(x)_{\text{numerical}}$
0.5	0.25	$10^{-1}$	0.36	1.1
0.5	0.25	$10^{-3}$	0.251001	1.001
0.5	0.25	$10^{-6}$	0.250001000001	1.000001

**Water Mass**

$$\frac{\partial \phi (s_l \rho_l X_w^l + s_g \rho_g X_w^g)}{\partial t} = -\nabla \cdot (\rho_l X_w^l \mathbf{q}_l + \rho_g X_w^g \mathbf{q}_g + \mathbf{J}_w^l + \mathbf{J}_w^g) + q_w$$

**Air Mass**

$$\frac{\partial \phi (s_l \rho_l X_a^l + s_g \rho_g X_a^g)}{\partial t} = -\nabla \cdot (\rho_l X_a^l \mathbf{q}_l + \rho_g X_a^g \mathbf{q}_g + \mathbf{J}_a^l + \mathbf{J}_a^g) + q_a$$

**Energy**

$$\frac{\partial \phi (s_l \rho_l U_l + s_g \rho_g U_g) + (1 - \phi) C_p^{\text{rock}} \rho_{\text{rock}} T}{\partial t} = -\nabla \cdot (\rho_l H_l \mathbf{q}_l + \rho_g H_g \mathbf{q}_g - \kappa_{\text{eff}} \nabla T) + q_e$$

$\phi$  = effective porosity [-]

$s_l$  = liquid saturation [-]

$s_g$  = gas saturation [-]

$\rho_l$  = liquid phase density [kmol/m<sup>3</sup>]

$\rho_g$  = gas phase density [kmol/m<sup>3</sup>]

$X_w^l$  = mole fraction of water in the liquid phase [-]

$X_w^g$  = mole fraction of water in gas phase [-]

$X_a^l$  = mole fraction of air in the liquid phase [-]

$X_a^g$  = mole fraction of air in gas phase [-]

$\mathbf{q}_l$  = liquid phase Darcy flux [m/sec]

$\mathbf{q}_g$  = gas phase Darcy flux [m/sec]

$\mathbf{J}_w^l$  = water diffusive flux in liquid phase [kmol/m<sup>2</sup>/sec]

$\mathbf{J}_a^l$  = air diffusive flux in liquid phase [kmol/m<sup>2</sup>/sec]

$\mathbf{J}_w^g$  = water vapor diffusive flux in gas phase [kmol/m<sup>2</sup>/sec]

$\mathbf{J}_a^g$  = air diffusive flux in gas phase [kmol/m<sup>2</sup>/sec]

$q_w$  = water source/sink [kmol/sec]

$q_a$  = air source/sink [kmol/sec]

$q_e$  = energy source/sink [MJ/sec]

$U_l$  = liquid phase internal energy [MJ/kmol]

$U_g$  = gas phase internal energy [MJ/kmol]

$H_l$  = liquid phase enthalpy [MJ/kmol]

$H_g$  = gas phase enthalpy [MJ/kmol]

$C_p^{\text{rock}}$  = rock heat capacity [MJ/kg rock-K]

$\rho_{\text{rock}}$  = rock particle density [kg/m<sup>3</sup> rock]

$T$  = temperature [C]

$\kappa_{\text{eff}}$  = effective thermal conductivity [W/K-m]

*Darcy Flux*

$$\mathbf{q}_\alpha = -\frac{k k_\alpha}{\mu_\alpha} \nabla (p_\alpha - \gamma_\alpha g z), \quad (\alpha = l, g)$$

*Air Diffusion in Liquid Phase*

$$\mathbf{J}_a^l = -\tau \phi S_l D_l \rho_l \nabla X_a^l$$

*Air Diffusion in Gas Phase*

$$\mathbf{J}_a^g = -\tau \phi S_g D_g^0 \left( \frac{T}{T_K} \right)^\theta \frac{p_0}{p_g} \rho_g \nabla X_a^g$$

$\mathbf{q}_\alpha$  = Darcy flux for phase  $\alpha$  [m/s]

$k$  = intrinsic permeability [m<sup>2</sup>]

$k_\alpha$  = relative permeability for phase  $\alpha$  [-]

$\mu_\alpha$  = viscosity for phase  $\alpha$  [Pa-s]

$p_\alpha$  = pressure for phase  $\alpha$  [Pa]

$\gamma_\alpha$  = density for phase  $\alpha$  [kg/m<sup>3</sup>]

$g$  = gravity [m/s<sup>2</sup>]

$z$  = elevation [m]

$\mathbf{J}_a^l$  = diffusive flux of air in liquid phase [kmol/m<sup>2</sup>-s]

$\tau$  = tortuosity [-]

$D_l$  = aqueous diffusivity [m<sup>2</sup>/s]

$\mathbf{J}_a^g$  = diffusive flux of air in gas phase [kmol/m<sup>2</sup>-s]

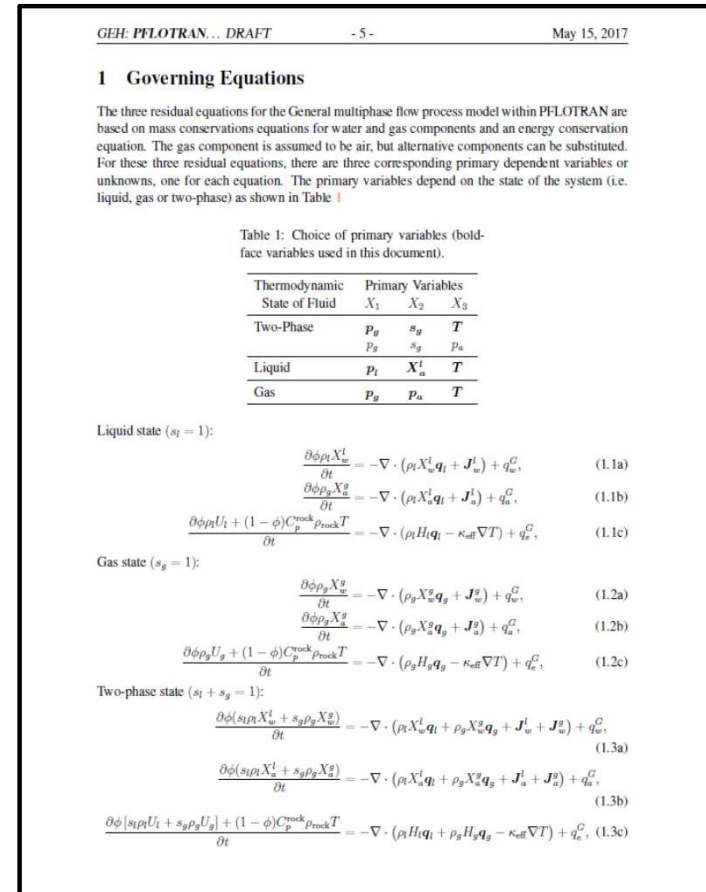
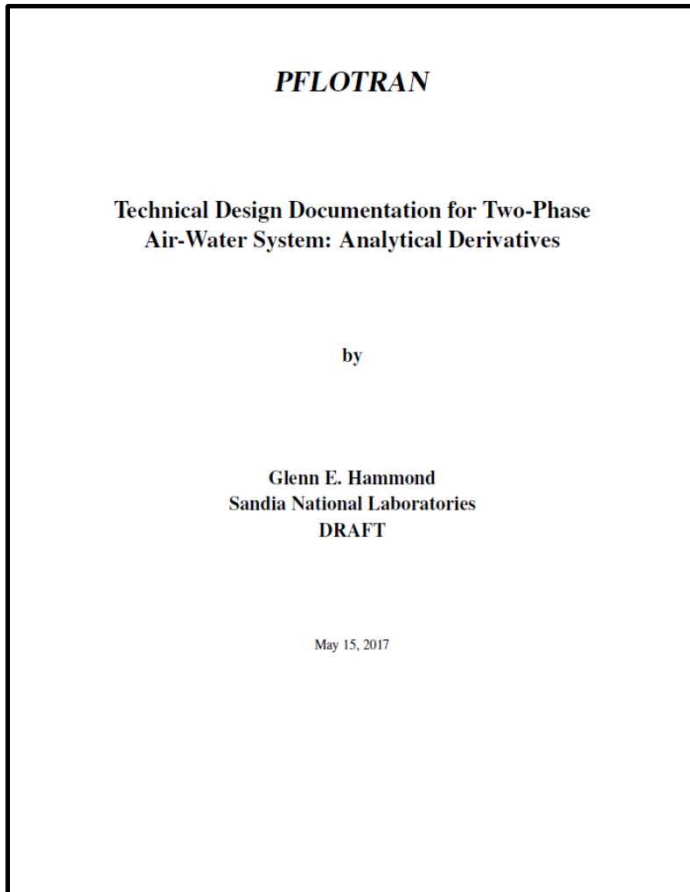
$D_g^0$  = gas diffusivity [m<sup>2</sup>/s]

$p_0$  = reference pressure [Pa]

## Primary Dependent Variables for Each Thermodynamic State

Thermodynamic State of Fluid	Primary Variables		
	$X_1$	$X_2$	$X_3$
Liquid	$p_l$	$X_a^l$	$T$
Gas	$p_g$	$p_a$	$T$
Two-Phase	$p_g$	$s_g$	$T$

> 38 pages of derivatives



# Table of Derivatives

Variable	State								
	Liquid			Gas			Two Phase		
	$p_l$	$X_a^l$	$T$	$p_g$	$p_a$	$T$	$p_g$	$s_g$	$T$
$p_l$	—						X	X	
$p_g$				—			—		
$p_a$					—		X		X
$p_c$								X	
$p_v$				X	X				X
$p_s$						X			X
$s_l$								X	
$s_g$								—	
$K_H$						X			X
$\rho_l$	X		X				X		X
$\rho_g$				X	X	X	X		X
$T$			—			—			—
$H_l$	X		X				X		X
$H_g$				X	X	X	X		X
$H_v$				X	X	X			X
$H_a$					X	X	X		X
$U_l$	X		X				X		X
$U_g$				X	X	X	X		X
$U_v$				X	X	X			X
$U_a$					X	X	X		X
$\rho_v$				X	X	X			X
$\rho_a$					X	X	X		X
$X_w^l$		X					X		X
$X_a^l$		—					X		X
$X_w^g$				X	X		X		X
$X_a^g$				X	X		X		X
$\mu_l$	X		X				X		X
$\mu_g$				X	X	X	X		X
$k_{rl}$								X	
$k_{rg}$								X	
$\phi$	X		X	X		X	X		X

$$\begin{aligned}
 & \frac{V}{\Delta t} \left[ (\phi(s_l \rho_l X_w^l + s_g \rho_g X_w^g))^{k+1} - (\phi(s_l \rho_l X_w^l + s_g \rho_g X_w^g))^k \right] \\
 & - \sum A \rho_l X_w^l \frac{k k_l}{\mu_l} \left( \frac{p_l^{i+1} - p_l^i}{\Delta x} - \gamma_l g z \right) \\
 & - \sum A \rho_g X_w^g \frac{k k_g}{\mu_g} \left( \frac{p_g^{i+1} - p_g^i}{\Delta x} - \gamma_g g z \right) \\
 & - \sum A \tau \phi s_l D_l \rho_l \left( \frac{X_w^{l\ i+1} - X_w^{l\ i}}{\Delta x} \right) \\
 & - \sum A \tau \phi s_g D_g^0 \left( \frac{T}{T_K} \right)^\theta \frac{p_0}{p_g} \rho_g \left( \frac{X_w^{g\ i+1} - X_w^{g\ i}}{\Delta x} \right) \\
 & - q_w = 0
 \end{aligned}$$

# Discrete Form of Water Mass Conservation Equation

$$\frac{V}{\Delta t} \left[ (\phi(s_l \rho_l X_w^l + s_g \rho_g X_w^g))^{k+1} - (\phi(s_l \rho_l X_w^l + s_g \rho_g X_w^g))^k \right]$$

$$- \sum A \rho_l X_w^l \frac{k k_l}{\mu_l} \left( \frac{p_l^{i+1} - p_l^i}{\Delta x} - \gamma_l g z \right)$$

$$- \sum A \rho_g X_w^g \frac{k k_g}{\mu_g} \left( \frac{p_g^{i+1} - p_g^i}{\Delta x} - \gamma_g g z \right)$$

$$- \sum A \tau \phi s_l D_l \rho_l \left( \frac{X_w^{l\ i+1} - X_w^{l\ i}}{\Delta x} \right)$$

$$- \sum A \tau \phi s_g D_g^0 \left( \frac{T}{T_K} \right)^\theta \frac{p_0}{p_g} \rho_g \left( \frac{X_w^{g\ i+1} - X_w^{g\ i}}{\Delta x} \right)$$

$$- q_w = 0$$

Variables with derivatives with respect to gas pressure are in *red*.

# Derivative of Water Equation Darcy Flux with Respect to Gas Pressure

$$\begin{aligned}
 \frac{\partial F_{w,i}^{\text{Darcy}}}{\partial p_{g,\text{up}}} = & -A_i \left( \rho_l p_{g,\text{up}} X_w^l \frac{kk_{rl}}{\mu_l} \left( \frac{p_{l,\text{dn}} - p_{l,\text{up}} - \gamma_l \cdot \mathbf{x}}{\Delta x} \right) + \right. \\
 & \rho_l X_{wp_{g,\text{up}}}^l \frac{kk_{rl}}{\mu_l} \left( \frac{p_{l,\text{dn}} - p_{l,\text{up}} - \gamma_l \cdot \mathbf{x}}{\Delta x} \right) + \\
 & \rho_l X_w^l \left( -\frac{kk_{rl}}{\mu_l^2} \mu_l p_{g,\text{up}} \right) \left( \frac{p_{l,\text{dn}} - p_{l,\text{up}} - \gamma_l \cdot \mathbf{x}}{\Delta x} \right) + \\
 & \rho_l X_w^l \frac{kk_{rl}}{\mu_l} \left( \frac{-p_{l,\text{up}} p_{g,\text{up}} - \gamma_l p_{g,\text{up}} \cdot \mathbf{x}}{\Delta x} \right) + \\
 & \rho_g p_{g,\text{up}} X_w^g \frac{kk_{rg}}{\mu_g} \left( \frac{p_{g,\text{dn}} - p_{g,\text{up}} - \gamma_g \cdot \mathbf{x}}{\Delta x} \right) + \\
 & \rho_g X_{wp_{g,\text{up}}}^g \frac{kk_{rg}}{\mu_g} \left( \frac{p_{g,\text{dn}} - p_{g,\text{up}} - \gamma_g \cdot \mathbf{x}}{\Delta x} \right) + \\
 & \rho_g X_w^g \left( -\frac{kk_{rg}}{\mu_g^2} \mu_g p_{g,\text{up}} \right) \left( \frac{p_{g,\text{dn}} - p_{g,\text{up}} - \gamma_g \cdot \mathbf{x}}{\Delta x} \right) + \\
 & \left. \rho_g X_w^g \frac{kk_{rg}}{\mu_g} \left( \frac{-1 - \gamma_g p_{g,\text{up}} \cdot \mathbf{x}}{\Delta x} \right) \right)
 \end{aligned}$$

Derivatives with respect to gas pressure are in red.

# Discrete Form of Water Mass Conservation Equation

$$\frac{V}{\Delta t} \left[ (\phi(s_l \rho_l X_w^l + s_g \rho_g X_w^g))^{k+1} - (\phi(s_l \rho_l X_w^l + s_g \rho_g X_w^g))^k \right]$$

$$- \sum A \rho_l X_w^l \frac{k k_l}{\mu_l} \left( \frac{p_l^{i+1} - p_l^i}{\Delta x} - \gamma_l g z \right)$$

$$- \sum A \rho_g X_w^g \frac{k k_g}{\mu_g} \left( \frac{p_g^{i+1} - p_g^i}{\Delta x} - \gamma_g g z \right)$$

$$- \sum A \tau \phi s_l D_l \rho_l \left( \frac{X_w^{l\ i+1} - X_w^{l\ i}}{\Delta x} \right)$$

$$- \sum A \tau \phi s_g D_g^0 \left( \frac{T}{T_K} \right)^\theta \frac{p_0}{p_g} \rho_g \left( \frac{X_w^{g\ i+1} - X_w^{g\ i}}{\Delta x} \right)$$

$$- q_w = 0$$

Variables with derivatives with respect to gas saturation are in *red*.

# Derivative of Water Equation Darcy Flux with Respect to Gas Pressure

$$\begin{aligned} \frac{\partial F_{w,i}^{\text{Darcy}}}{\partial s_{gup}} = & -A_i \left( \rho_l X_w^l \frac{k k_{rl} s_{gup}}{\mu_l} \left( \frac{p_{l,dn} - p_{l,up} - \gamma_l \cdot \mathbf{x}}{\Delta x} \right) + \right. \\ & \left. \rho_l X_w^l \frac{k k_{rl}}{\mu_l} \left( \frac{-p_{l,up} s_{gup}}{\Delta x} \right) + \right. \\ & \left. \rho_g X_w^g \frac{k k_{rg} s_{gup}}{\mu_g} \left( \frac{p_{g,dn} - p_{g,up} - \gamma_g \cdot \mathbf{x}}{\Delta x} \right) \right) \end{aligned}$$

*Derivatives with respect to gas saturation are in red.*

# Derivative of Water Equation Darcy Flux wrt. Gas Pressure, Gas Saturation and Temperature

## Derivative wrt. gas pressure

$$\begin{aligned} \frac{\partial F_{w,i}^{\text{Darcy}}}{\partial p_{g,\text{up}}} = & -A_i \left( \rho_l p_{g,\text{up}} X_w^l \frac{k k_{rl}}{\mu_l} \left( \frac{p_{l,\text{dn}} - p_{l,\text{up}} - \gamma_l \cdot \mathbf{x}}{\Delta x} \right) + \right. \\ & \rho_l X_w^l \frac{k k_{rl}}{\mu_l} \left( \frac{p_{l,\text{dn}} - p_{l,\text{up}} - \gamma_l \cdot \mathbf{x}}{\Delta x} \right) + \\ & \rho_l X_w^l \left( -\frac{k k_{rl}}{\mu_l^2} \mu_l p_{g,\text{up}} \right) \left( \frac{p_{l,\text{dn}} - p_{l,\text{up}} - \gamma_l \cdot \mathbf{x}}{\Delta x} \right) + \\ & \rho_l X_w^l \frac{k k_{rl}}{\mu_l} \left( \frac{-p_{l,\text{up}} p_{g,\text{up}} - \gamma_l p_{g,\text{up}} \cdot \mathbf{x}}{\Delta x} \right) + \\ & \rho_g p_{g,\text{up}} X_w^g \frac{k k_{rg}}{\mu_g} \left( \frac{p_{g,\text{dn}} - p_{g,\text{up}} - \gamma_g \cdot \mathbf{x}}{\Delta x} \right) + \\ & \rho_g X_w^g \frac{k k_{rg}}{\mu_g} \left( \frac{p_{g,\text{dn}} - p_{g,\text{up}} - \gamma_g \cdot \mathbf{x}}{\Delta x} \right) + \\ & \rho_g X_w^g \left( -\frac{k k_{rg}}{\mu_g^2} \mu_g p_{g,\text{up}} \right) \left( \frac{p_{g,\text{dn}} - p_{g,\text{up}} - \gamma_g \cdot \mathbf{x}}{\Delta x} \right) + \\ & \left. \rho_g X_w^g \frac{k k_{rg}}{\mu_g} \left( \frac{-1 - \gamma_g p_{g,\text{up}} \cdot \mathbf{x}}{\Delta x} \right) \right) \end{aligned}$$

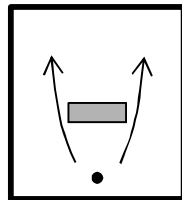
## Derivative wrt. gas saturation

$$\begin{aligned} \frac{\partial F_{w,i}^{\text{Darcy}}}{\partial s_{g,\text{up}}} = & -A_i \left( \rho_l X_w^l \frac{k k_{rl} s_{g,\text{up}}}{\mu_l} \left( \frac{p_{l,\text{dn}} - p_{l,\text{up}} - \gamma_l \cdot \mathbf{x}}{\Delta x} \right) + \right. \\ & \rho_l X_w^l \frac{k k_{rl}}{\mu_l} \left( \frac{-p_{l,\text{up}} s_{g,\text{up}}}{\Delta x} \right) + \\ & \left. \rho_g X_w^g \frac{k k_{rg} s_{g,\text{up}}}{\mu_g} \left( \frac{p_{g,\text{dn}} - p_{g,\text{up}} - \gamma_g \cdot \mathbf{x}}{\Delta x} \right) \right) \end{aligned}$$

## Derivative wrt. temperature

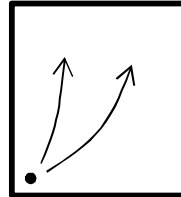
$$\begin{aligned} \frac{\partial F_{w,i}^{\text{Darcy}}}{\partial T_{\text{up}}} = & -A_i \left( \rho_l T_{\text{up}} X_w^l \frac{k k_{rl}}{\mu_l} \left( \frac{p_{l,\text{dn}} - p_{l,\text{up}} - \gamma_l \cdot \mathbf{x}}{\Delta x} \right) + \right. \\ & \rho_l X_w^l \frac{k k_{rl}}{\mu_l} \left( \frac{p_{l,\text{dn}} - p_{l,\text{up}} - \gamma_l \cdot \mathbf{x}}{\Delta x} \right) + \\ & \rho_l X_w^l \left( -\frac{k k_{rl}}{\mu_l^2} \mu_l T_{\text{up}} \right) \left( \frac{p_{l,\text{dn}} - p_{l,\text{up}} - \gamma_l \cdot \mathbf{x}}{\Delta x} \right) + \\ & \rho_l X_w^l \frac{k k_{rl}}{\mu_l} \left( \frac{-\gamma_l T_{\text{up}} \cdot \mathbf{x}}{\Delta x} \right) + \\ & \rho_g T_{\text{up}} X_w^g \frac{k k_{rg}}{\mu_g} \left( \frac{p_{g,\text{dn}} - p_{g,\text{up}} - \gamma_g \cdot \mathbf{x}}{\Delta x} \right) + \\ & \rho_g X_w^g \frac{k k_{rg}}{\mu_g} \left( \frac{p_{g,\text{dn}} - p_{g,\text{up}} - \gamma_g \cdot \mathbf{x}}{\Delta x} \right) + \\ & \rho_g X_w^g \left( -\frac{k k_{rg}}{\mu_g^2} \mu_g T_{\text{up}} \right) \left( \frac{p_{g,\text{dn}} - p_{g,\text{up}} - \gamma_g \cdot \mathbf{x}}{\Delta x} \right) + \\ & \left. \rho_g X_w^g \frac{k k_{rg}}{\mu_g} \left( \frac{-\gamma_g T_{\text{up}} \cdot \mathbf{x}}{\Delta x} \right) \right) \end{aligned}$$

*Gas Injection*



$\ R\ ^2$	Analytical				Numerical			
	Tol.	TS	NI	Cuts	Time [s]	TS	NI	Cuts
1e-8	185	576	7	1.36	185	577	7	1.99
5e-9	185	593	7	1.35	185	595	7	1.97
2e-9	179	581	5	1.42	179	583	5	1.97
1.5e-9	211	818	14	1.78	206	770	13	2.46
1e-9	206	770	13	1.86	425	1877	51	5.65
5e-10	211	837	14	1.82	Did not finish			

WIPP Case 5



$\ R\ ^2$	Analytical				Numerical			
Tol.	TS	NI	Cuts	Time [s]	TS	NI	Cuts	Time [s]
1e-8	88	277	0	1.52	88	227	0	2.17
1e-9	605	2939	135	1.65	702	3512	158	2.90

10.8M Grid Cells  
32.7M Unknowns  
1024 Processes

## *Multiphase Flow*

	<b>Time Step</b>	<b>Newton It.</b>	<b>Linear It.</b>	<b>Cuts</b>	<b>Time [h]</b>
Analytical	684	2790	544,632	61	1.37
Numerical	1617	6003	3293	85	4.05

## *Reactive Transport*

	<b>Time Step</b>	<b>Newton It.</b>	<b>Linear It.</b>	<b>Cuts</b>	<b>Time [h]</b>
Analytical	684	1478	17623	0	1.06
Numerical	1617	3293	30305	0	1.91

# Spent Fuel and Waste Science and Technology

# Analytical vs. Numerical Defense Waste Repository Simulation Output

```
== GENERAL FLOW ==
0 2r: 2.19E-08 2x: 0.00E+00 2u: 0.00E+00 ir: 4.49E-09 iu: 0.00E+00 rsn: 0
1 2r: 1.96E-12 2x: 1.97E+10 2u: 2.78E+02 ir: 3.79E-14 iu: 2.58E+00 rsn: 0
2 2r: 4.48E-13 2x: 1.97E+10 2u: 3.88E-01 ir: 3.88E-15 iu: 3.62E-02 rsn: itol_p
ost_check

Step 684 Time= 1.00000E+06 Dt= 2.57624E+02 [y] snes_conv_reason: 12
newton = 2 [ 2790] linear = 647 [ 544632] cuts = 0 [ 61]
--> SNES Linear/Non-Linear Iterations = 647 / 2
--> SNES Residual: 4.479497E-13 4.112524E-20 3.880035E-15
--> max chng: dpl= 2.5836E+00 dpq= 0.0000E+00 dpa= 0.0000E+00
dxa= 1.3279E-10 dt= 8.5261E-04 dsg= 0.0000E+00

== REACTIVE TRANSPORT ==
0 2r: 3.03E-11 2x: 0.00E+00 2u: 0.00E+00 ir: 1.61E-12 iu: 0.00E+00 rsn: 0
1 2r: 6.58E-16 2x: 1.12E-03 2u: 1.02E-03 ir: 1.81E-16 iu: 6.11E-06 rsn: 0
2 2r: 4.49E-21 2x: 1.12E-03 2u: 9.30E-09 ir: 1.38E-21 iu: 3.58E-10 rsn: rtol

Step 684 Time= 1.00000E+06 Dt= 2.57624E+02 [y] snes_conv_reason: 3
newton = 2 [ 1478] linear = 15 [ 17623] cuts = 0 [ 0]
--> SNES Linear/Non-Linear Iterations = 15 / 2
--> SNES Residual: 4.492066E-21 4.124063E-28 1.377087E-21
--> max chng: dcmx= 1.1989E-17 dc/dt= 1.4757E-27 [mol/s]
dvfmx= 0.0000E+00 dvf/dt= 0.0000E+00 [1/s]

== WASTE FORM MODEL ==
== USED FUEL DISPOSITION DECAY MODEL ==
FLOW TS BE steps = 684 newton = 2790 linear = 544632 cuts = 61
FLOW TS BE Wasted Linear Iterations = 90235
FLOW TS BE SNES time = 4945.4 seconds

TRAN TS BE steps = 684 newton = 1478 linear = 17623 cuts = 0
TRAN TS BE Wasted Linear Iterations = 0
TRAN TS BE SNES time = 3828.0 seconds

Wall Clock Time: 9.3224E+03 [sec] 1.5537E+02 [min] 2.5895E+00 [hr]
```

```
== GENERAL FLOW ==
0 2r: 5.27E-09 2x: 0.00E+00 2u: 0.00E+00 ir: 9.50E-10 iu: 0.00E+00 rsn: 0
1 2r: 1.67E-10 2x: 1.97E+10 2u: 4.22E+01 ir: 1.38E-12 iu: 2.11E-01 rsn: 0
2 2r: 7.28E-10 2x: 1.97E+10 2u: 5.76E-01 ir: 3.53E-12 iu: 1.47E-02 rsn: 0
3 2r: 3.25E-12 2x: 1.97E+10 2u: 5.88E-02 ir: 1.73E-14 iu: 1.28E-04 rsn: 0
4 2r: 5.41E-13 2x: 1.97E+10 2u: 3.38E-04 ir: 5.67E-15 iu: 9.66E-06 rsn: atol

Step 1617 Time= 1.00000E+06 Dt= 5.46242E+02 [y] snes_conv_reason: 2
newton = 4 [ 6003] linear = 1188 [ 1692396] cuts = 0 [ 85]
--> SNES Linear/Non-Linear Iterations = 1188 / 4
--> SNES Residual: 5.413352E-13 4.969875E-20 5.673050E-15
--> max chng: dpl= 2.1116E-01 dpq= 0.0000E+00 dpa= 0.0000E+00
dxa= 2.0726E-12 dt= 1.9602E-04 dsg= 0.0000E+00

== REACTIVE TRANSPORT ==
0 2r: 2.84E-11 2x: 0.00E+00 2u: 0.00E+00 ir: 3.61E-13 iu: 0.00E+00 rsn: 0
1 2r: 3.16E-16 2x: 1.51E-03 2u: 1.40E-03 ir: 1.45E-16 iu: 7.15E-06 rsn: 0
2 2r: 7.20E-22 2x: 1.51E-03 2u: 1.44E-08 ir: 3.03E-22 iu: 2.48E-10 rsn: rtol

Step 1617 Time= 1.00000E+06 Dt= 5.46242E+02 [y] snes_conv_reason: 3
newton = 2 [ 3293] linear = 20 [ 30305] cuts = 0 [ 0]
--> SNES Linear/Non-Linear Iterations = 20 / 2
--> SNES Residual: 7.202834E-22 6.612758E-29 3.029625E-22
--> max chng: dcmx= 5.1129E-19 dc/dt= 2.9681E-29 [mol/s]
dvfmx= 0.0000E+00 dvf/dt= 0.0000E+00 [1/s]

== WASTE FORM MODEL ==
== USED FUEL DISPOSITION DECAY MODEL ==
FLOW TS BE steps = 1617 newton = 6003 linear = 1692396 cuts = 85
FLOW TS BE Wasted Linear Iterations = 71431
FLOW TS BE SNES time = 14591.8 seconds

TRAN TS BE steps = 1617 newton = 3293 linear = 30305 cuts = 0
TRAN TS BE Wasted Linear Iterations = 0
TRAN TS BE SNES time = 6862.5 seconds

Wall Clock Time: 2.2652E+04 [sec] 3.7753E+02 [min] 6.2921E+00 [hr]
```