

Simulator Overview
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PROCESS MODELING

PHYSICAL PROBLEM

- define model purpose
- define important processes
- appropriate level of complexity
- well defined simplifying assumptions and limitations

MATHEMATICAL INTERPRETATION OF THE PHYSICS

- reduce the physical system into a set of mathematical equations
- define mass balance equations
- define constitutive equations (models)
- definitive parameters must be able to be estimated at the appropriate scale

NUMERICAL (DISCRETE) REPRESENTATION

- computer solution
- accurate
- robust (solution efficiency)

PRE- AND POST-PROCESSING

- visualization
- presentation
- aid in model development

NAPL Simulator

OUTLINE:

Model purpose

Model Attributes (Physics)

Model Attributes (numerics)

Sensitive parameters

Model utility

Model Input and Output

Example problems

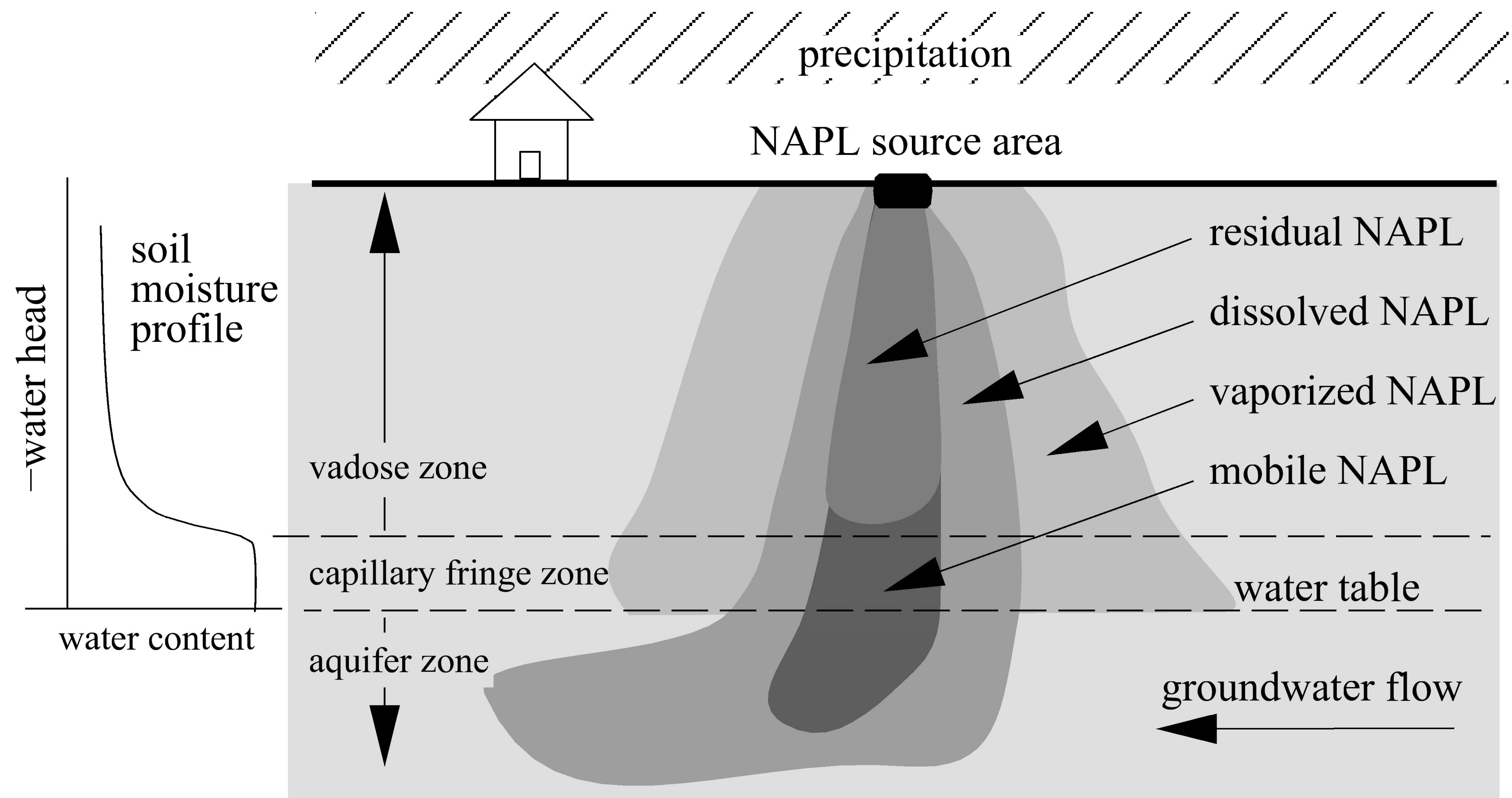
pre-processing with EXCEL

Model Purpose

- Research funded by EPA's Kerr Lab
- To develop a mathematical and numerical model capable of describing the migration and fate of NAPL's in variably liquid-saturated, near-surface, granular soils.
- To use this model to verify our understanding of the physical and chemical processes governing the flow and fate of NAPL contaminants.
- Simulate the artificial aquifer experiments being conducted at Kerr Lab (meter-scale).

Summary of Simulator Capabilities - Physics

- Consider one, two, or three spatial dimensions
- Consider one, two, or three-phase flow
- Consider fluid entrapment during drainage and release during imbibition.
- Consider hysteresis in the k-S-P relationship.
- Employ the wettability constraint, from most to least: water – NAPL - gas
- Consider rate-limited mass transfer to describe NAPL dissolution and vaporization
- Consider advective-dispersive transport of NAPL species in both the water and gas phases



Summary of Simulator Capabilities - Physics

- The **NAPL-phase**:
 - o made up of a single chemical species
 - o constant density and viscosity
 - o consider constant first order decay
 - o consider rate-limited dissolution mass transfer to and from the water-phase
 - o consider rate-limited vaporization mass transfer to and from the gas-phase
- The **Water-phase**:
 - o made up of two chemical species: water and dissolved NAPL
 - o density and viscosity a function of NAPL concentration only
 - o consider rate-limited mass transfer of dissolved NAPL to and from the NAPL-phase
 - o consider rate-limited vaporization mass transfer of dissolved NAPL to and from the gas-phase
 - o consider linear equilibrium adsorption mass transfer of dissolved NAPL to and from the solid-phase
 - o consider constant first order decay of dissolved NAPL
 - o consider advective-dispersive transport of dissolved NAPL

Summary of Simulator Capabilities - Physics

(continued)

- The **Gas-phase**:
 - o made up of two chemical species: gas and NAPL vapor
 - o density and viscosity a function of NAPL concentration only (i.e., incompressible)
 - o consider rate-limited vaporization mass transfer of dissolved NAPL to and from the water-phase
 - o consider rate-limited mass transfer of NAPL vapor to and from the NAPL-phase
 - o Darcy's Law can be used to model phase advection
 - o Fick's Law can be used to model diffusion processes.
 - o consider advective-dispersive transport of NAPL vapor
- The **Solid-phase**:
 - o considered non-deforming
 - o isotropic and in general heterogeneous in space
 - o made up of two species: solid and adsorbed NAPL
 - o consider linear equilibrium adsorption mass transfer of dissolved NAPL to and from the water-phase

3-Phase empirical model for k-S-P

1.) Wettability constraint – contact angle constrained such that fluid wettability follows:

most **WATER – NAPL – GAS** least

From this we have:

$$P_{cNW}(S_W),$$

$$P_{cGN}(S_T)$$

$$S_T = S_W + S_N \text{ (total wetting phase)}$$

$$k_{rW}(S_W)$$

$$k_{rN}(S_W, S_T)$$

behaves like a non-wetting phase when no gas present

behaves like a wetting phase when no water present

$$k_{rG}(S_T)$$

2.) algebraic constraint: $P_{cGW} = P_{cNW} + P_{cGN}$

3.) scaling constraint: recall Laplace's equation: $P_{cGW} = \gamma_{GW} 2 / R^*$

$$\frac{P_{cGW}}{\gamma_{GW}} = \frac{P_{cNW}}{\gamma_{NW}} = \frac{P_{cGN}}{\gamma_{GN}}$$

4.) For equations 2 and 3 to hold : $\gamma_{GW} - \gamma_{NW} - \gamma_{GN} = 0$ (neutral spreading coefficient)

<p>RESULT: Same model to model 1, 2, or 3-phase flow, regardless of phase configuration</p>
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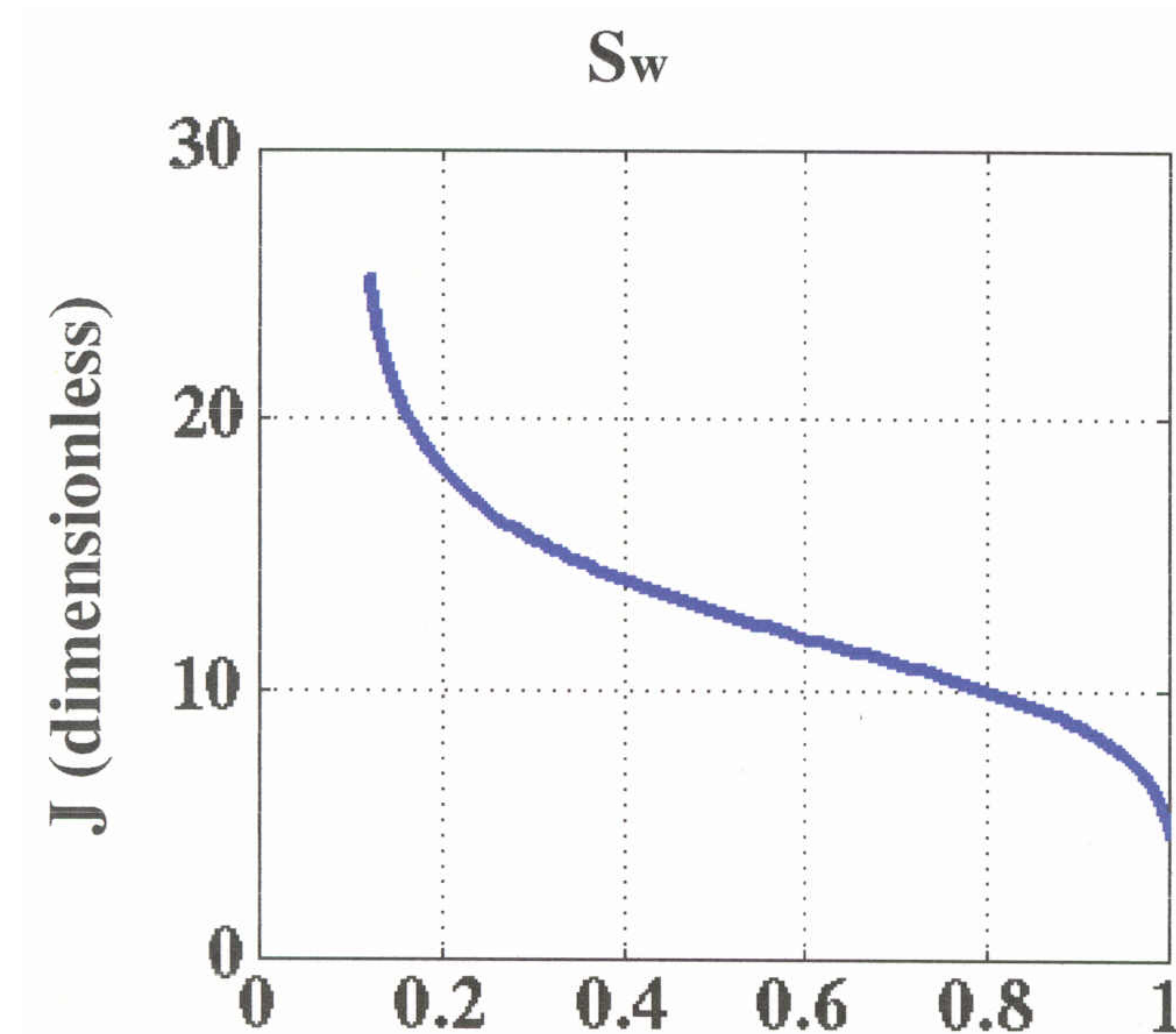
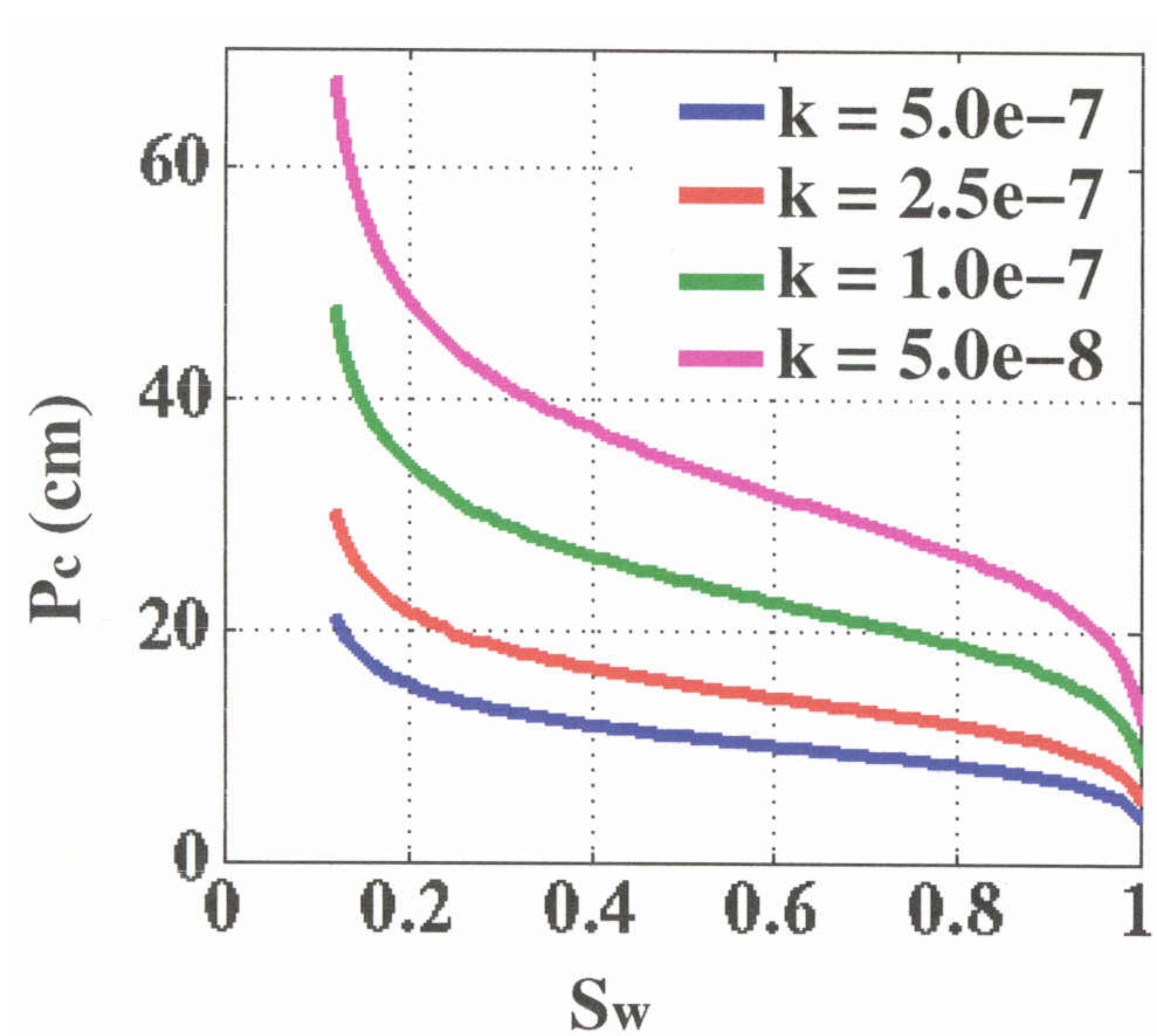
3-Phase empirical model for k-S-P

5.) Scaling for soil properties

recall Laplace's equation: $P_{cGW} = \gamma_{GW} \cdot 2 / R^*$

Leverett (1941) noted: $R^* / 2 \sim [k / \epsilon]^{1/2}$ shape of the interface is related to surface area

Therefore, define a dimensionless function: $J = P_{cGW} / \gamma_{GW} \cdot [k / \epsilon]^{1/2}$



3-Phase empirical model for k-S-P

Implications of physical and model constraints:

Benefits:

- Same model to model 1, 2, or 3-phase flow, regardless of phase configuration
- need to measure S-P relation for one phase pair. The other two functions are defined from:

$$\frac{P_{cGW}}{\gamma_{GW}} = \frac{P_{cNW}}{\gamma_{NW}} = \frac{P_{cGN}}{\gamma_{GN}}$$

(see next slide)

- Measure S-P for one soil type, and scale it for others (optional way to include heterogeneity)

Costs:

- Wetting constraint: water – NAPL – gas
- neutral spreading coefficient constraint (issue modeling chlorinated solvents)
- only two of the three fluid pair IFT values are independent ($\gamma_{GW} - \gamma_{NW} - \gamma_{GN} = 0$)

Example of Pc scaling based on IFT

e.g., W-G measured, therefore,

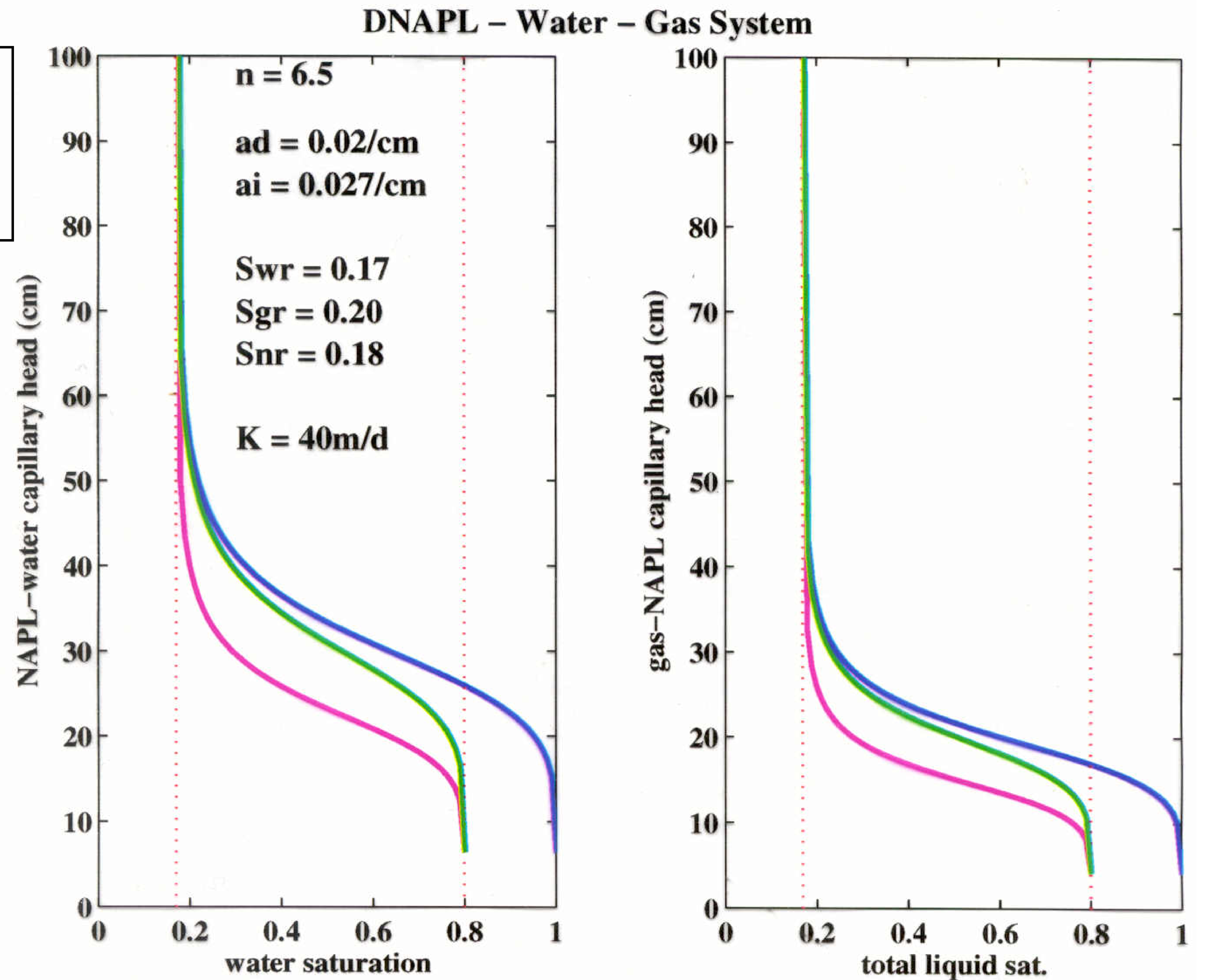
$$P_{cGW} \frac{\gamma_{GN}}{\gamma_{GW}} = P_{cGN}$$

$$P_{cGW} \frac{\gamma_{NW}}{\gamma_{GW}} = P_{cNW}$$

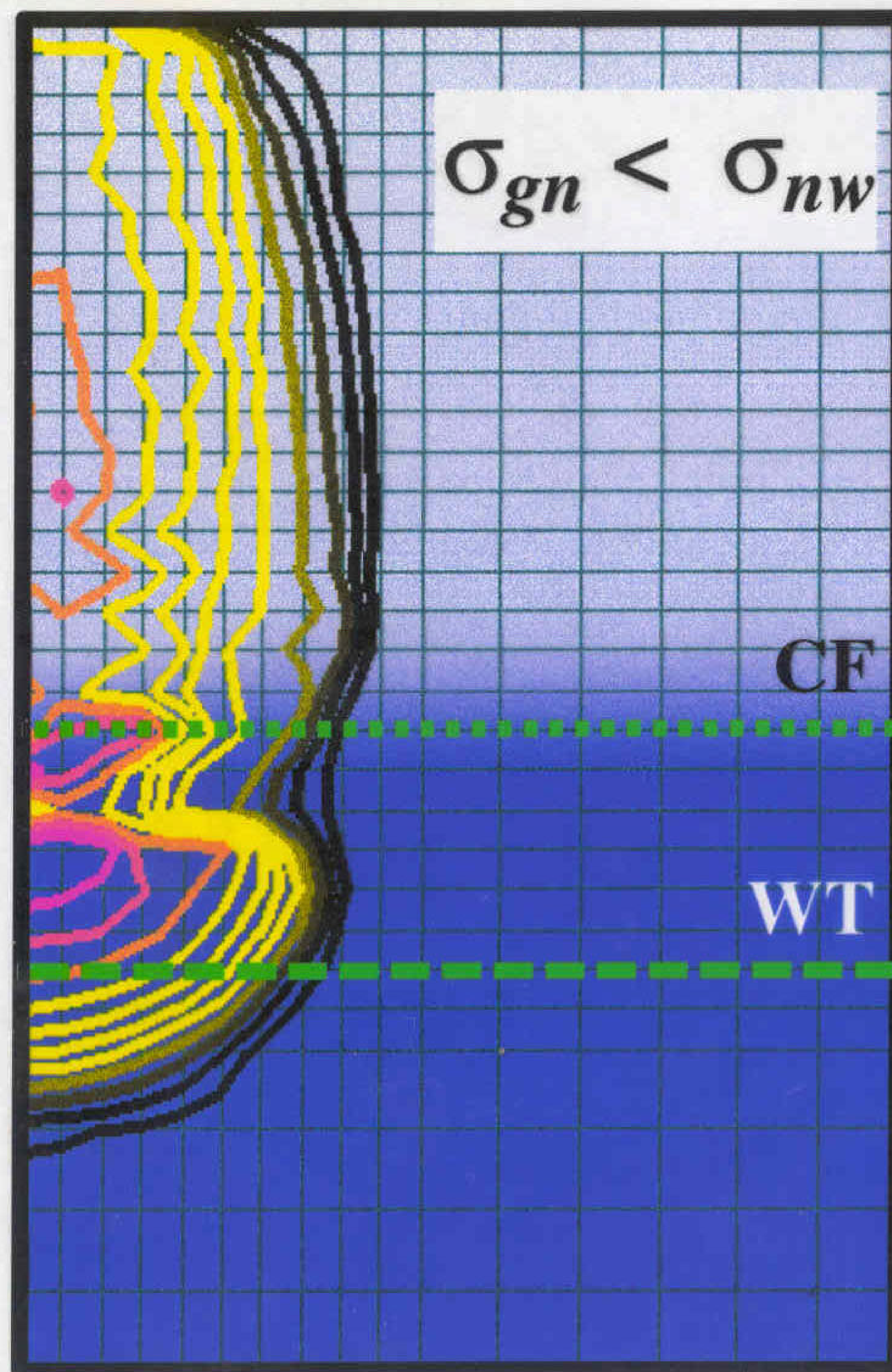
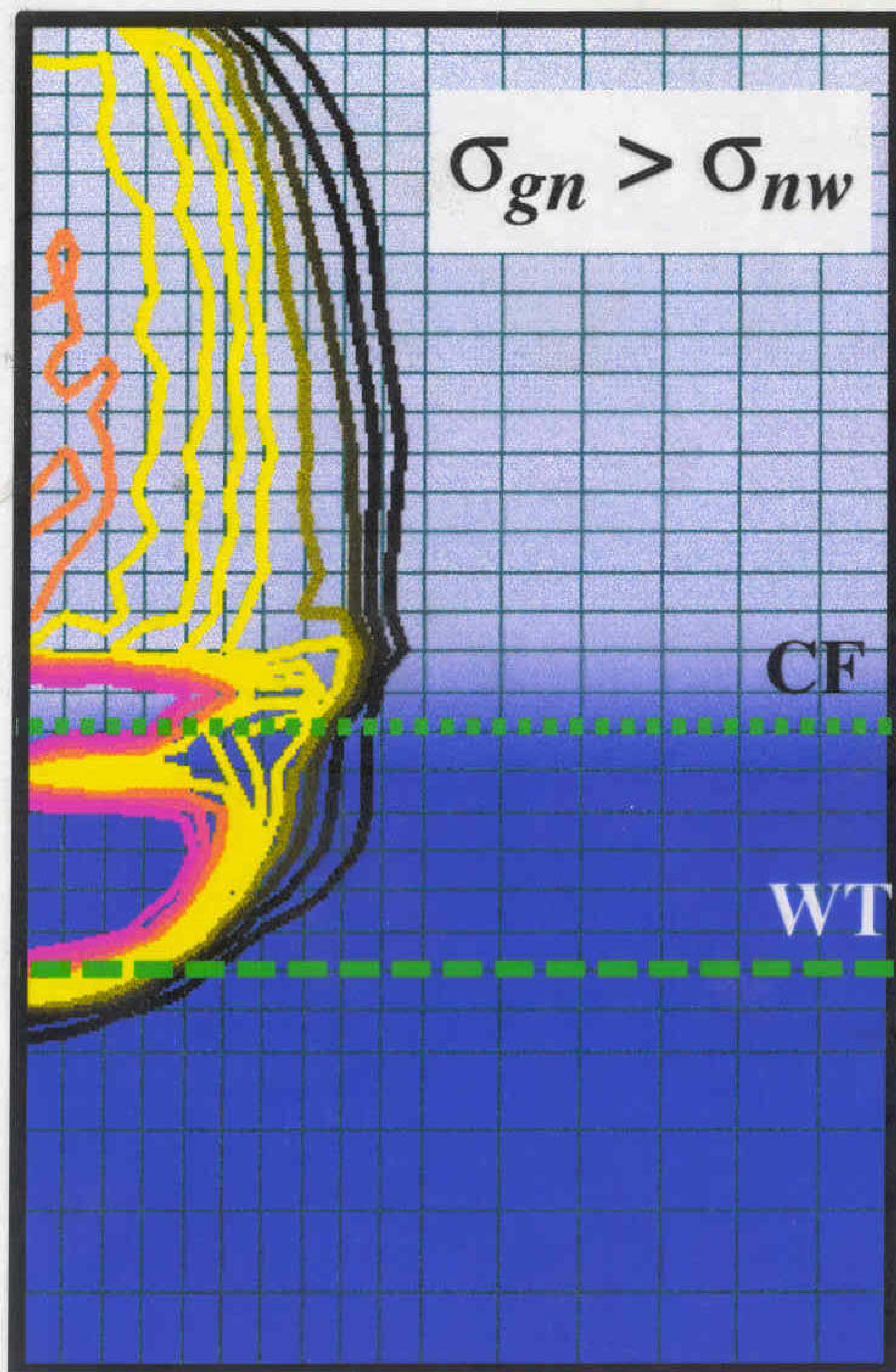
$$\gamma_{GW} = 73 \text{ dynes /cm}$$

$$\gamma_{NW} = 40 \text{ dynes /cm}$$

$$\gamma_{GN} = 32 \text{ dynes /cm}$$



$$\frac{P_{cgw}}{\sigma_{gw}} = \frac{P_{cnw}}{\sigma_{nw}} = \frac{P_{cgn}}{\sigma_{gn}}$$



S_N

0.100

0.0910

0.0820

0.0730

0.0640

0.0550

0.0460

0.0370

0.0280

0.0190

0.0100

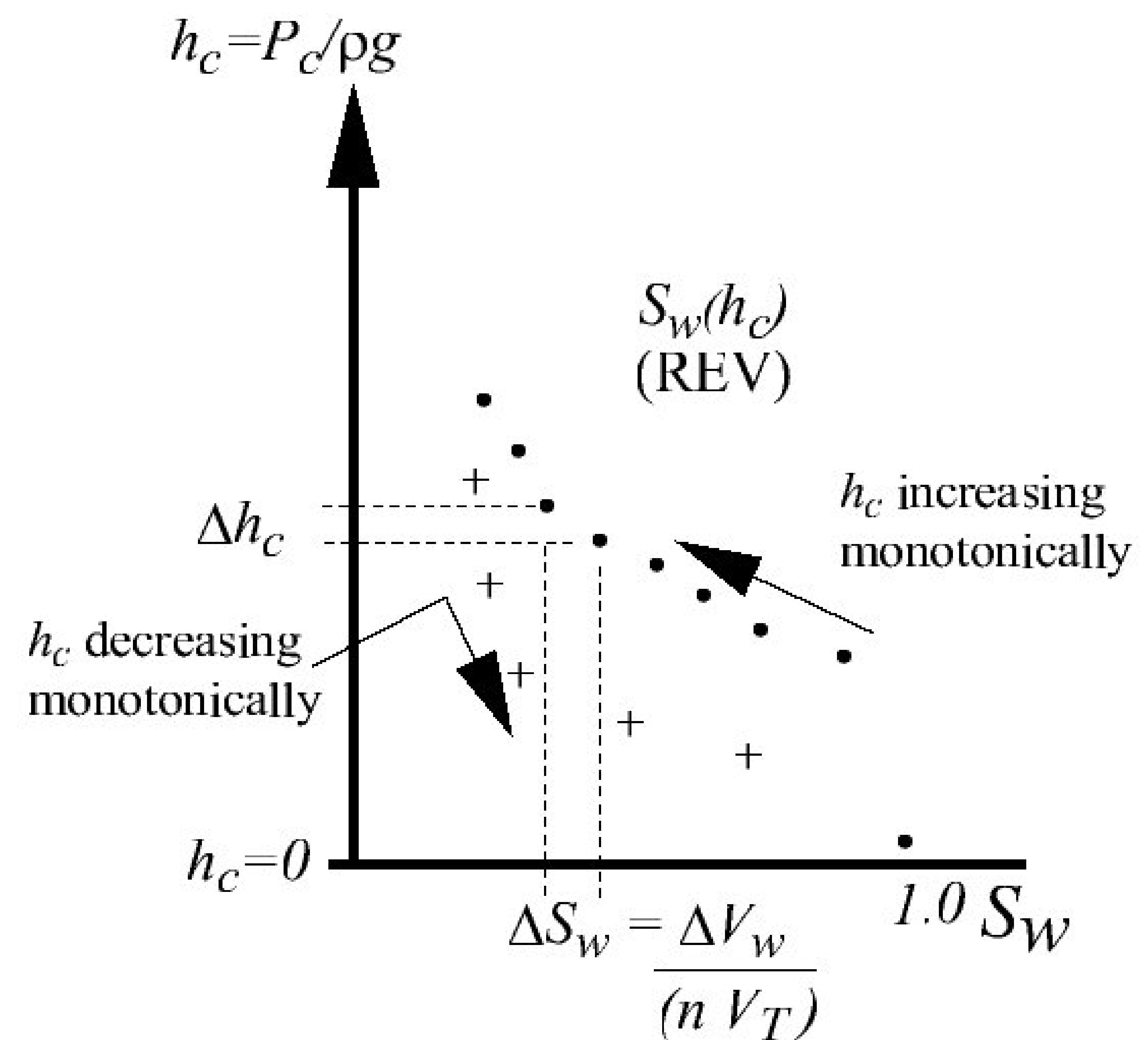
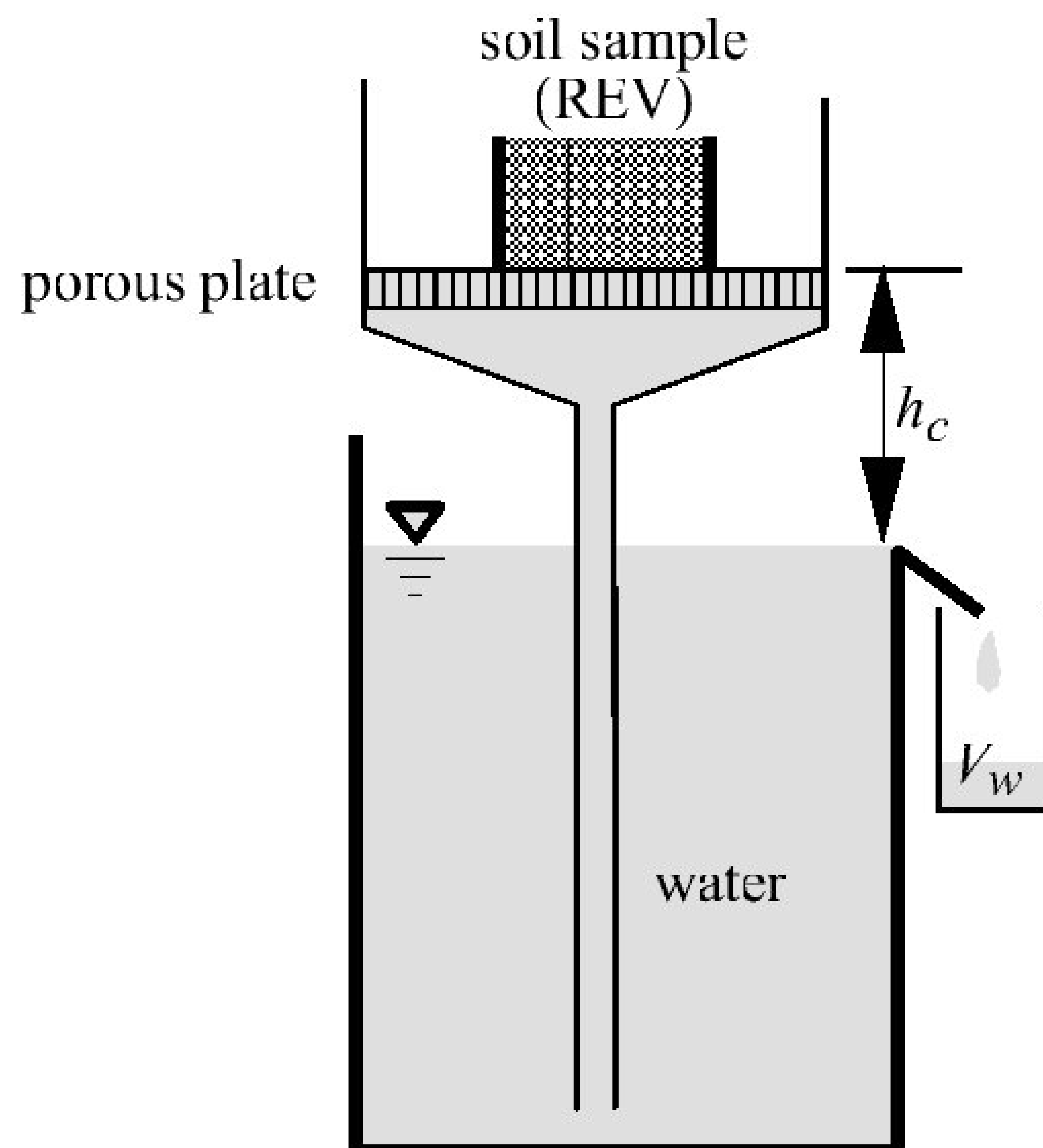
Hysteresis in k-S-P

Hysteresis in S-P primarily due to

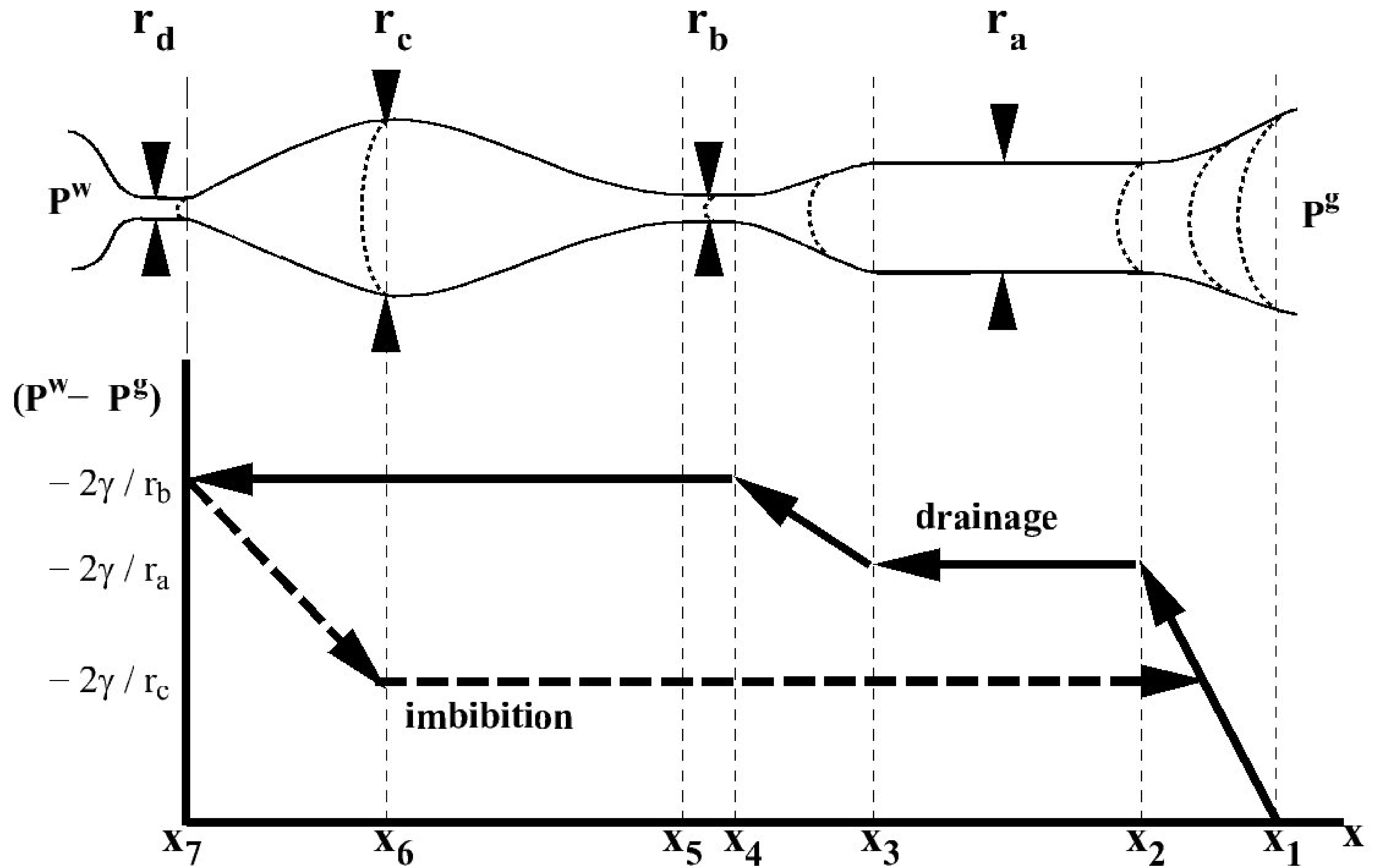
- capillary effects
- fluid entrapment effects

Hysteresis in k-S primarily due to

- fluid entrapment effects



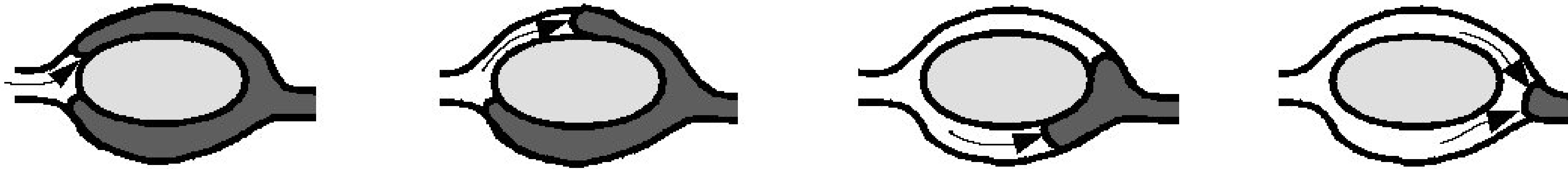
Capillary Hysteresis –



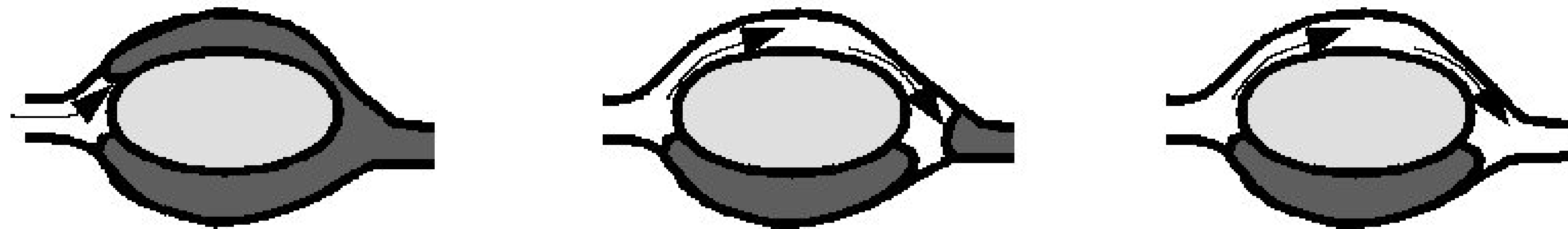
Pore throats control wetting phase drainage, pore bodies control wetting phase imbibition

Non-wetting-phase entrapment due to snap-off and by-passing

a.) stable displacement – no trapping



b.) trapping via by-passing



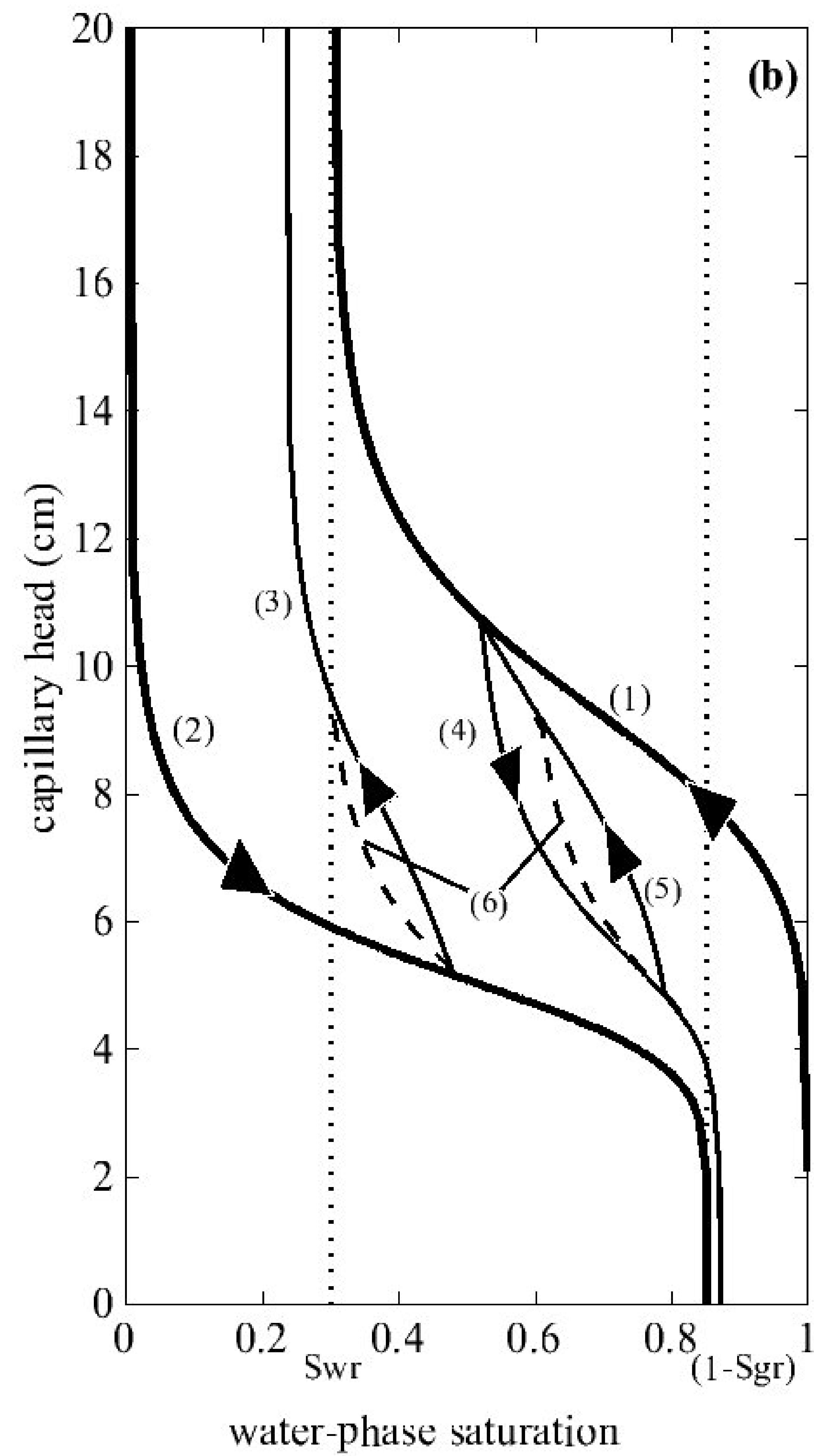
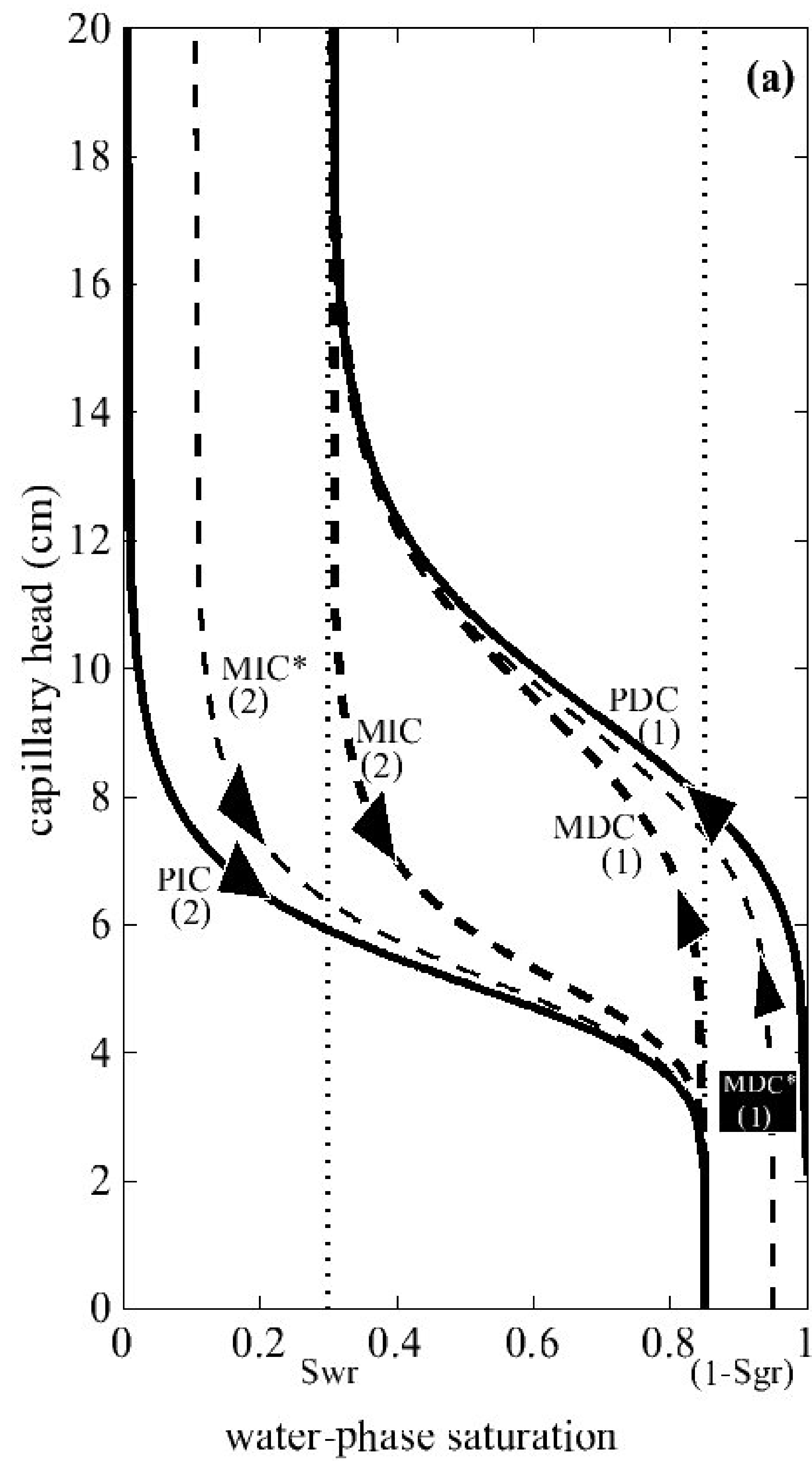
c.) trapping via by-passing and snap-off



Preferential flow:

Non-wetting phase prefers larger pores
Wetting phase prefers smaller pores.

Capillary and entrapment hysteresis (the S-P model used in the simulator)

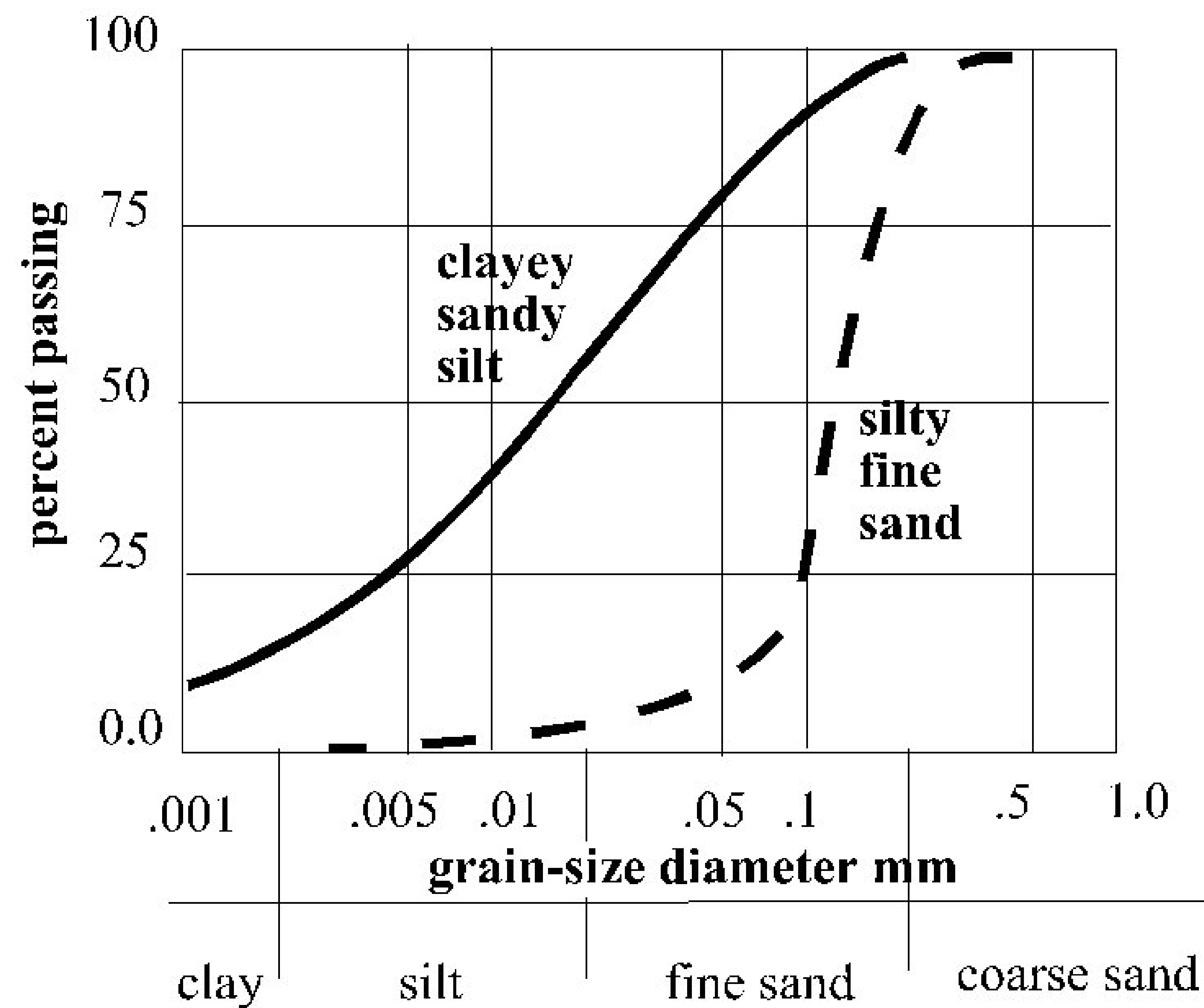


S-P is related to pore size distribution

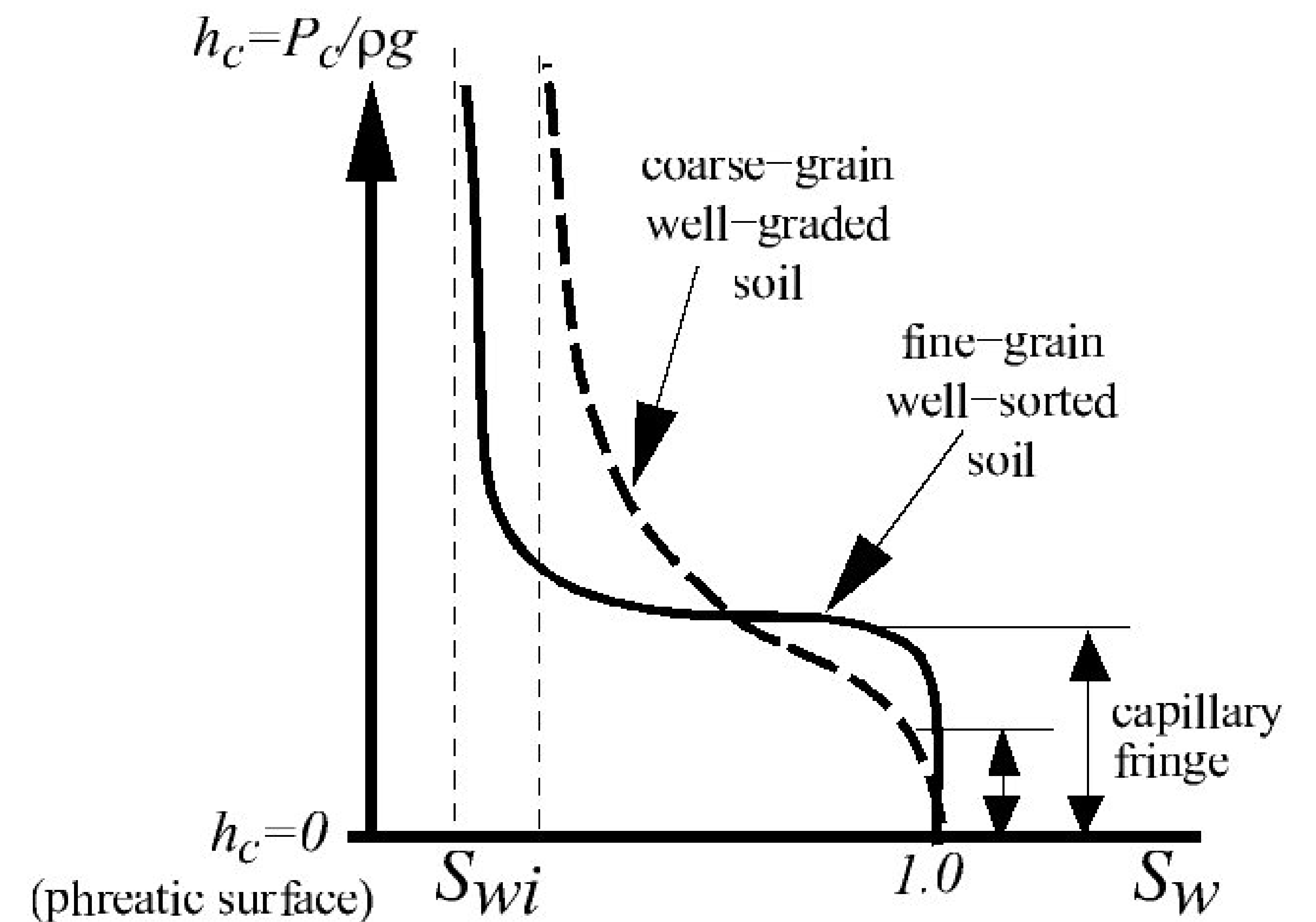
Pore size distribution is related to grain size distribution

Therefore, S-P is related to grain size distribution

Grain size distribution curves



Primary drainage curves



van Genuchten S-P model adapted to capillary and entrapment hysteresis

$$h_c(S_e) = \left[(S_e)^{-1/m} - 1 \right]^{1/\eta} (a)^{-1}$$

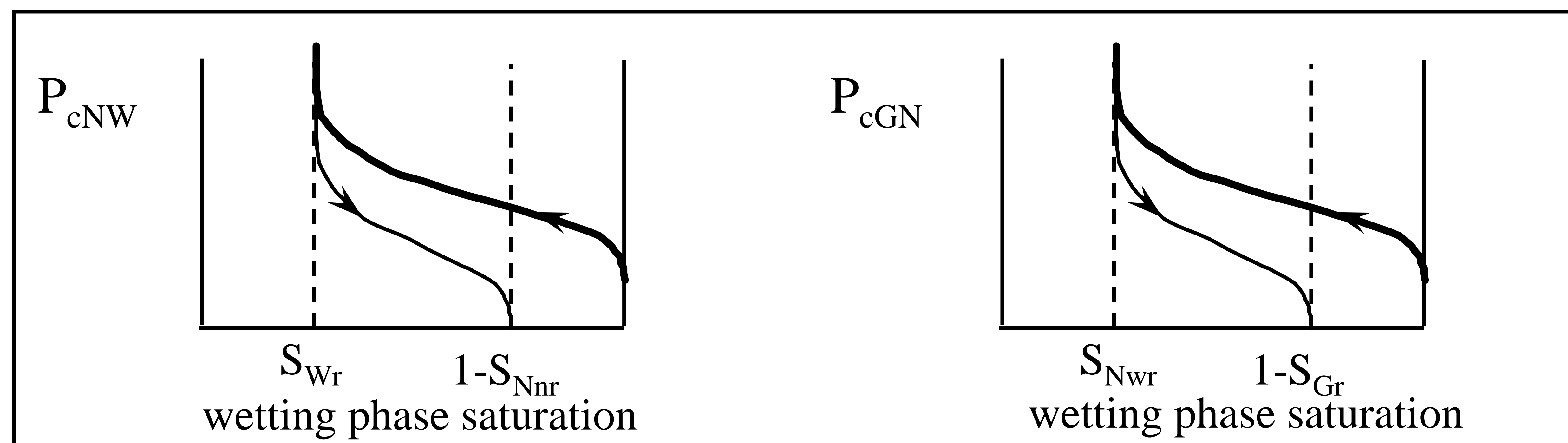
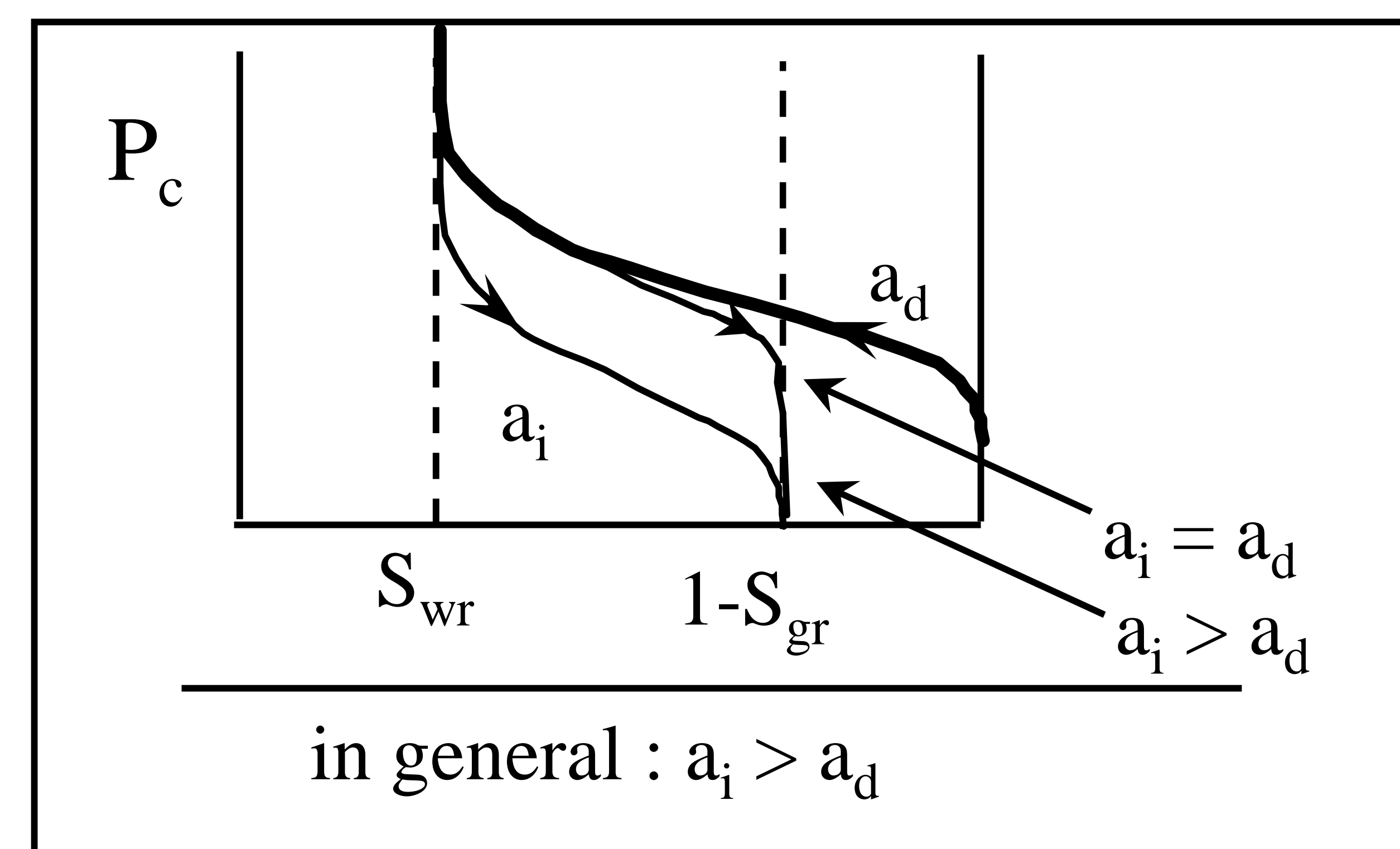
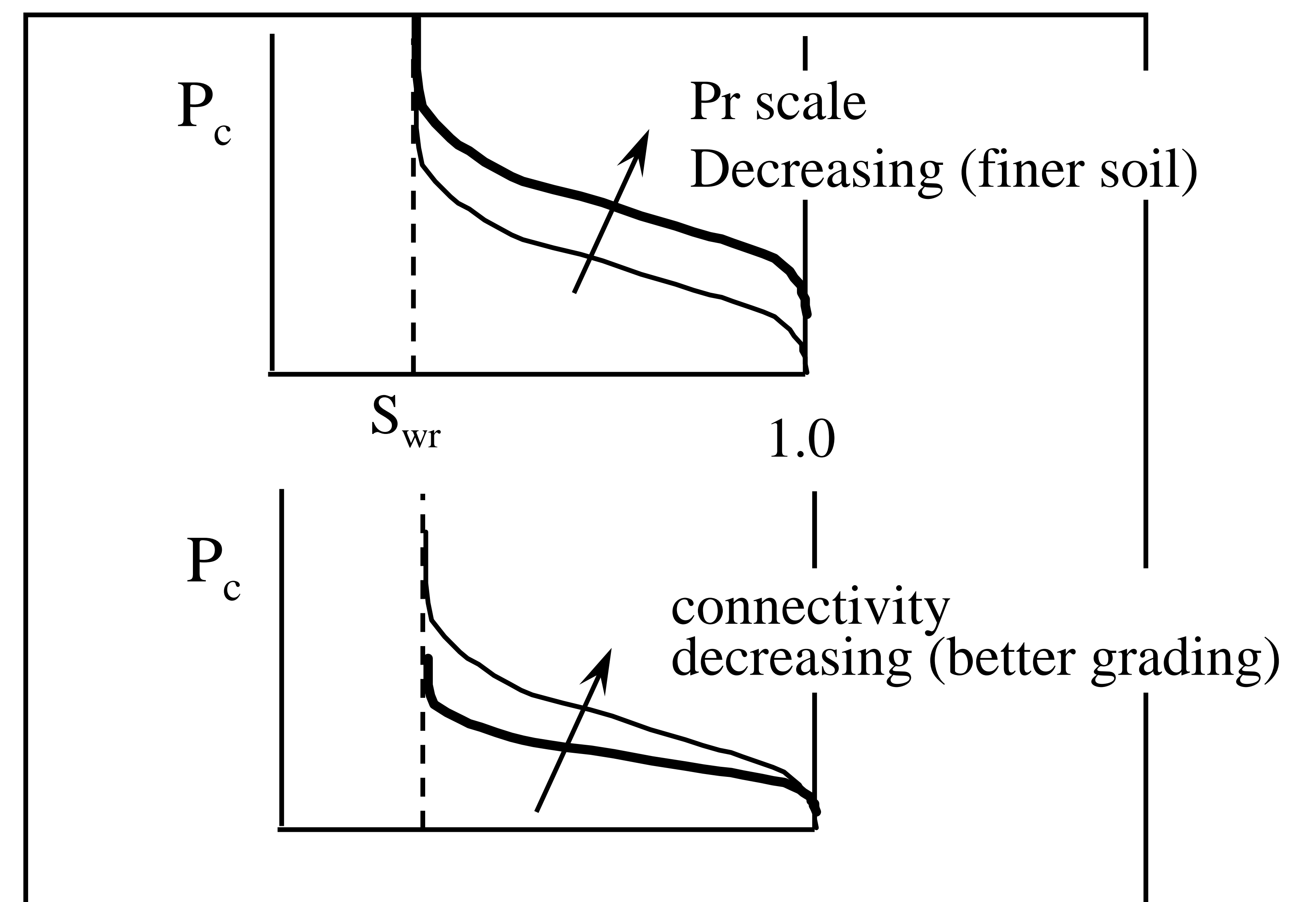
$$S_e = \frac{S_w - S_r}{S_s - S_r}, \quad 0 \leq S_e \leq 1$$

$$h_c = P_c / (\rho^w g)$$

a [1/L] – defines the pressure scale
 η Pore connectivity
 $m = 1 - 1/\eta$

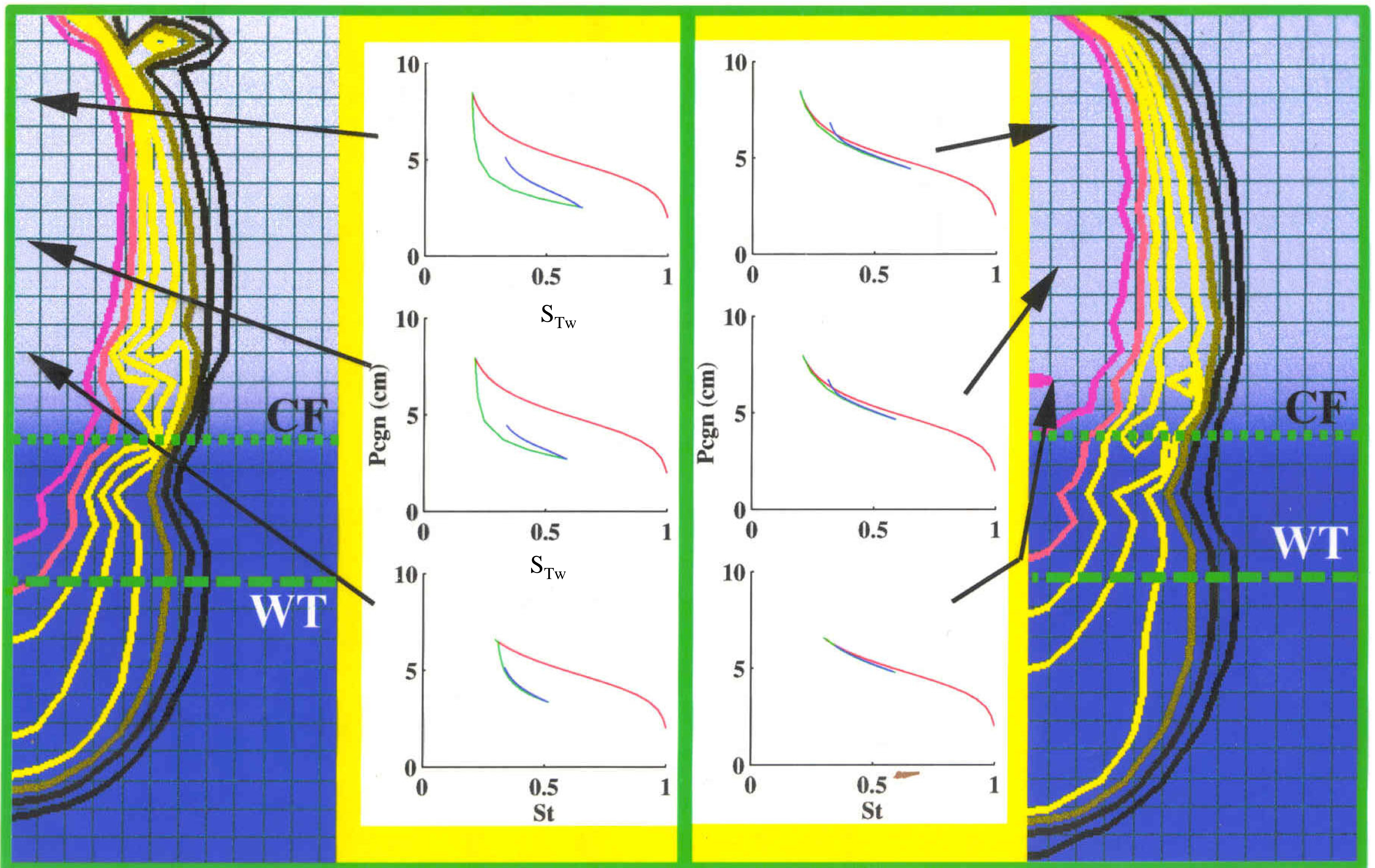
a is different for drainage (a_d)
 imbibition (a_i)

$S_s - S_r$ range over which two phase flow occurs
 (a function of phase entrapment)



$$a_i = 2 a_d$$

$$a_i = a_d$$



van Genuchten k-S model adapted to entrapment hysteresis

NOTE: assume that k_r is related to pore size distribution. Therefore, when no data are available, use the S-P model (also related to pore size distribution) to functionalize k-S.

$$k_{rW}(S_W) = ({}^a S_{eW})^\zeta \left\{ 1 - \left[1 - ({}^b S_{eW})^{1/m} \right]^m \right\}^2$$

$$k_{rG}(S_G) = ({}^a S_{eG})^\varphi \left[1 - \left[1 - ({}^b S_{eG}) \right]^{1/m} \right]^{2m}$$

$$k_{rN}(S_W, S_G) = (S_{eN})^\xi \left\{ \left[1 - (1 - S_{eTn})^{1/m} \right]^m - \left[1 - (S_{eTw})^{1/m} \right]^m \right\}^2$$

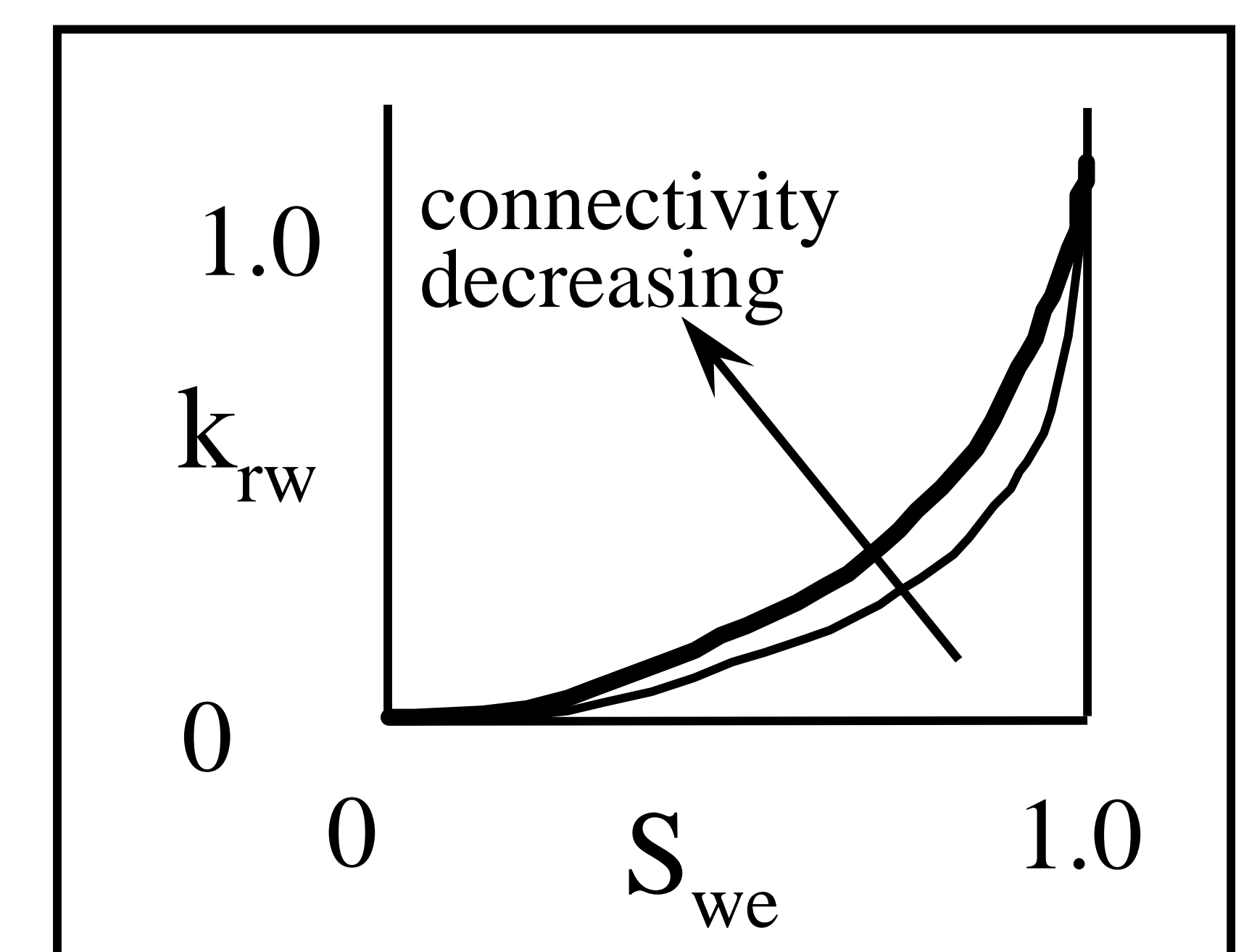
$$m = 1 - 1/\eta$$

η same as for S-P model

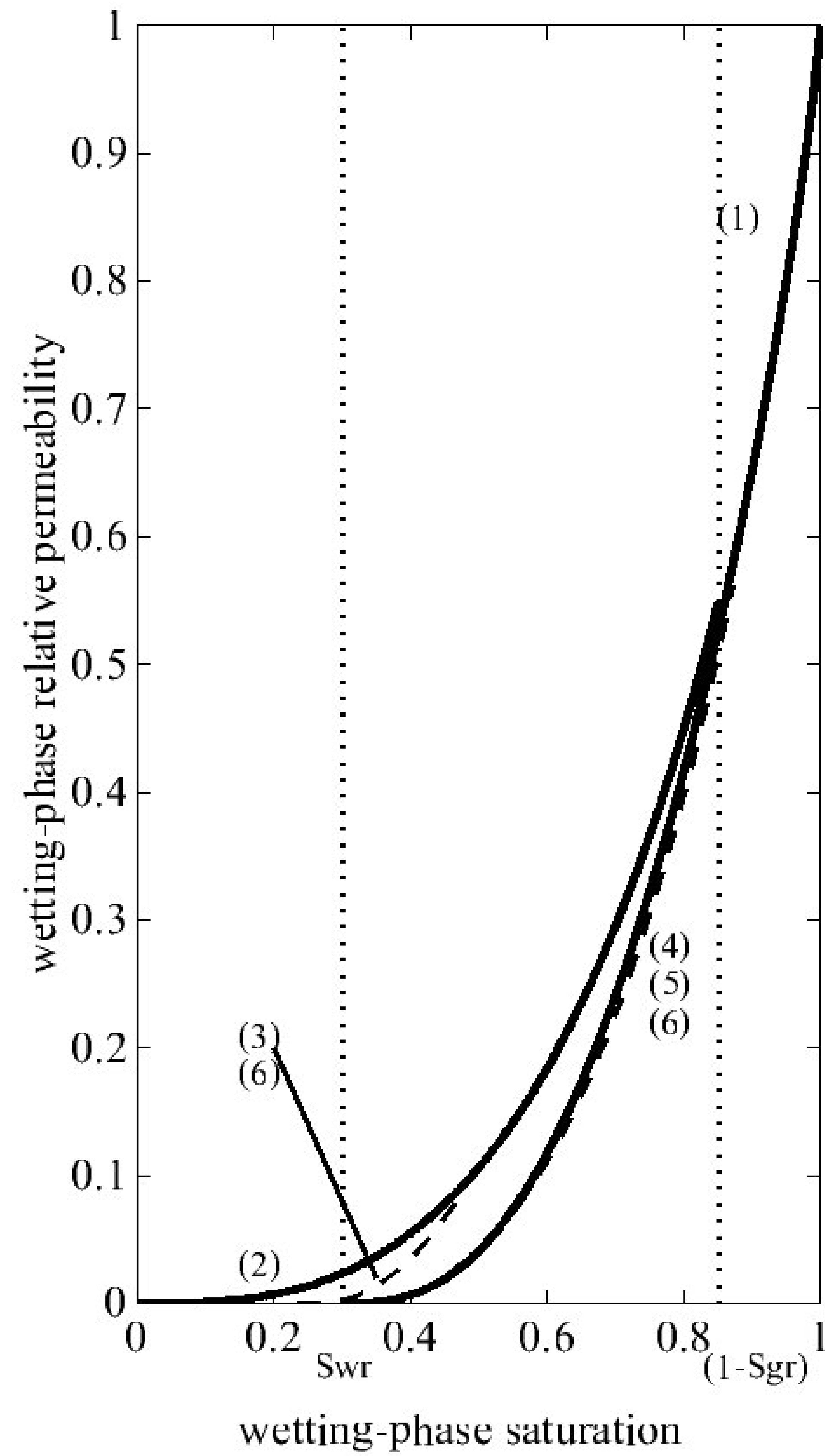
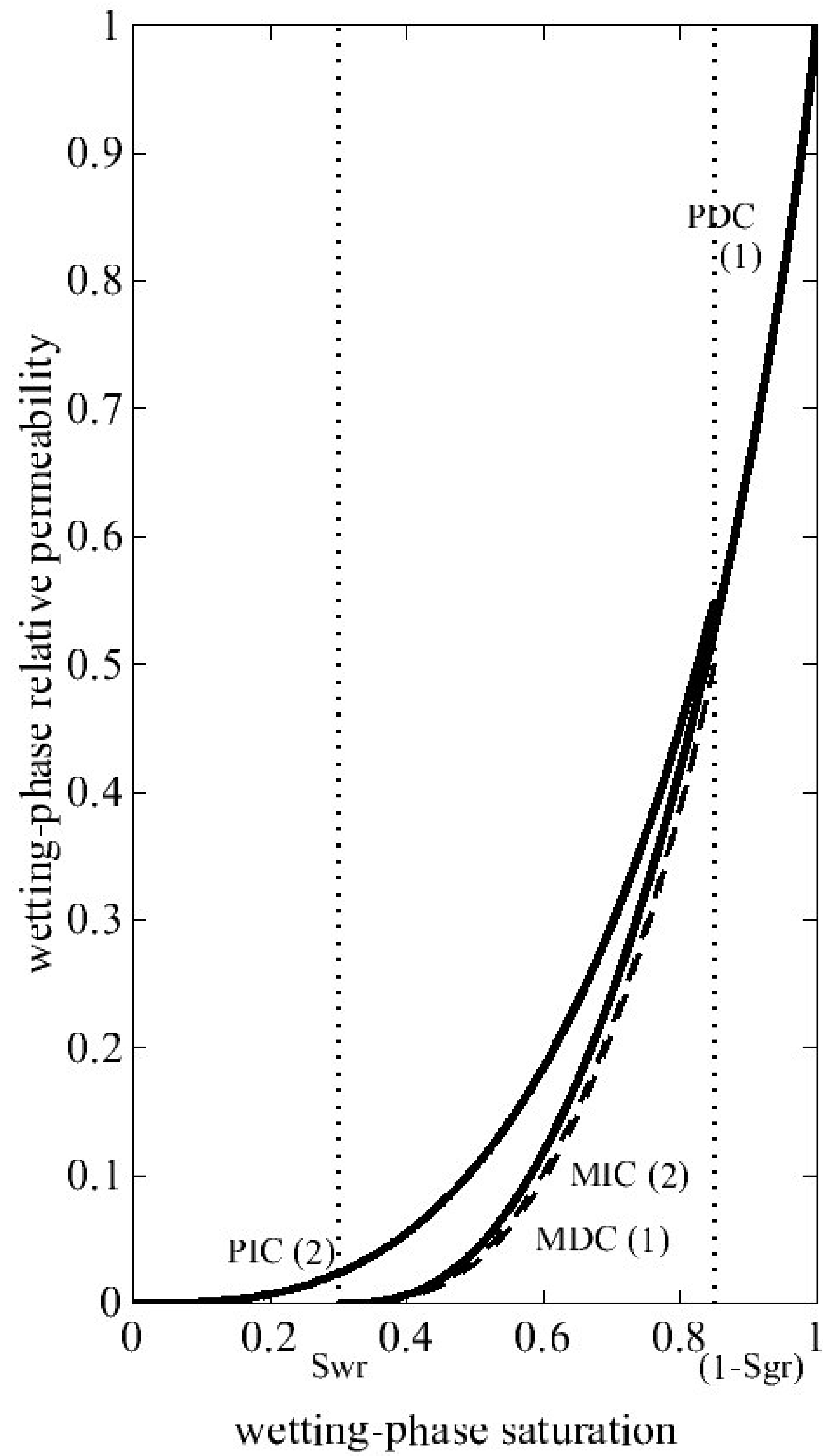
$S_e =$ effective saturation (range between 0 and 1)

Saturation scaled by the range over which the phase is mobile
(a function of phase entrapment)

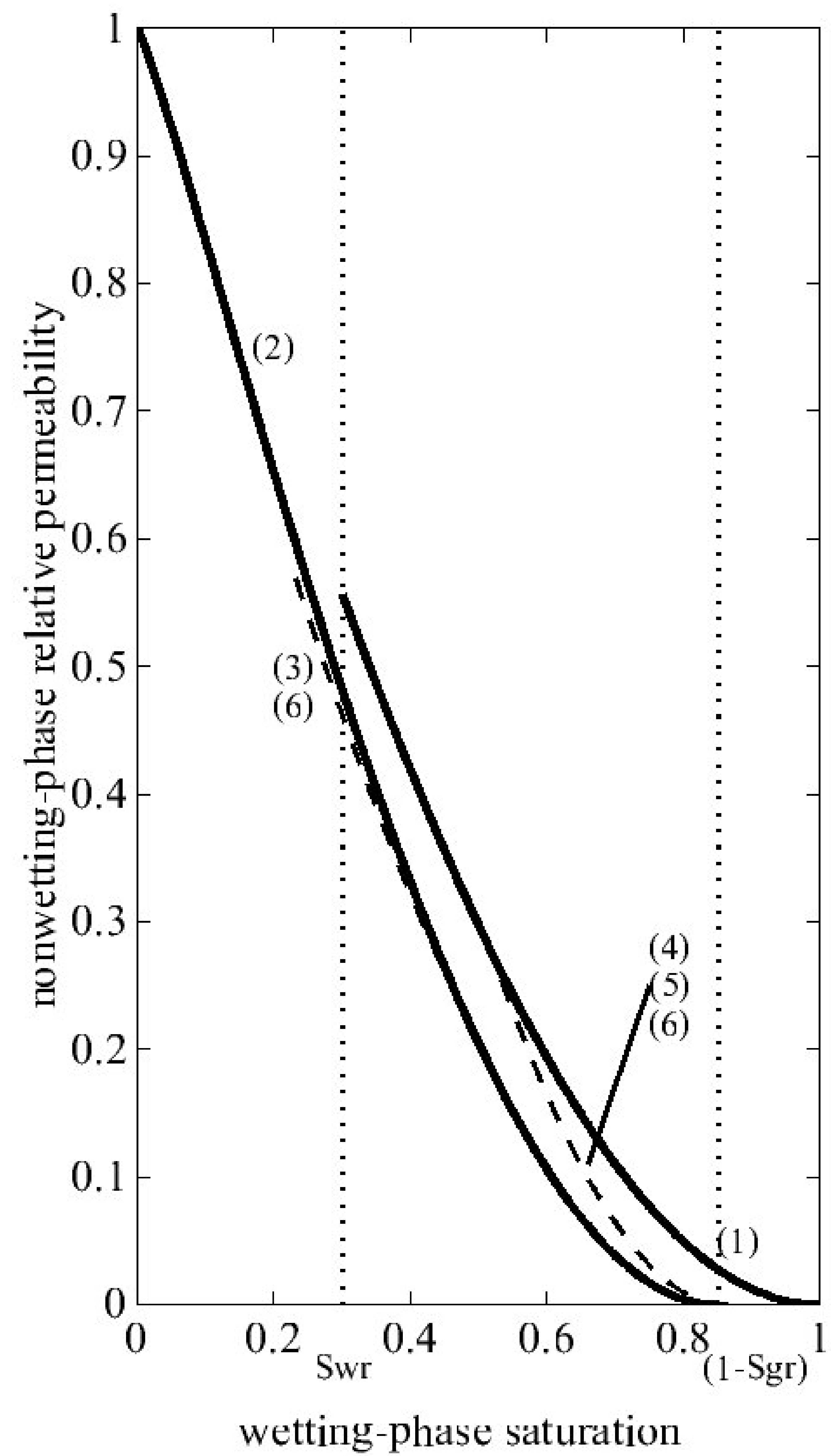
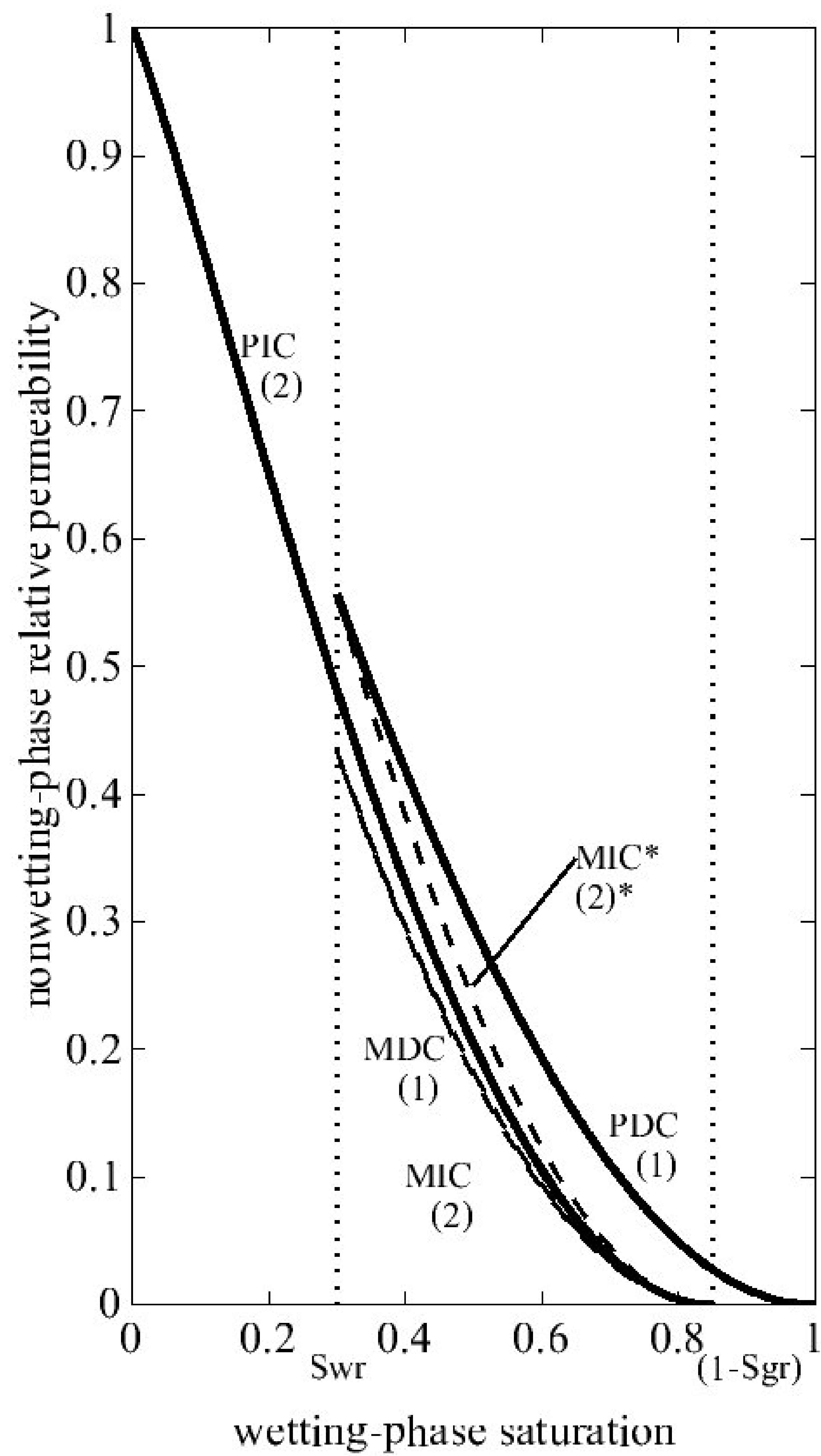
Power terms (ζ , φ , ξ) = pore connectivity (can be positive or negative, and in general connectivity for the wetting phase is larger than that for the non-wetting phase).



$k_{rw}(S_w)$ – corresponding to S-P curves shown previously



$k_{rN}(S_W)$ – corresponding to S-P curves shown previously



Summary Governing Equations

Consider 3-phase flow with constant fluid properties and without mass exchange

(3) Mass balance
equations

$$\begin{aligned}\varepsilon \partial S_W / \partial t + \nabla \cdot \mathbf{q}^W &= Q^W \\ \varepsilon \partial S_N / \partial t + \nabla \cdot \mathbf{q}^N &= Q^N \\ \varepsilon \partial S_G / \partial t + \nabla \cdot \mathbf{q}^G &= Q^G\end{aligned}$$

(1) Material balance

$$S_W + S_N + S_G = 1$$

(3) Darcy's Law

$$\begin{aligned}\mathbf{q}^W &= -\lambda^W (\nabla P^W - \rho^W \mathbf{g} \nabla D) \\ \mathbf{q}^N &= -\lambda^N (\nabla P^N - \rho^N \mathbf{g} \nabla D) \\ \mathbf{q}^G &= -\lambda^G (\nabla P^G - \rho^G \mathbf{g} \nabla D)\end{aligned}$$

$$\lambda^\alpha = k k_{r\alpha} / \mu^\alpha \text{ (phase mobility)}$$

(2) Saturation-Pressure
Relationships

$$\begin{aligned}P^N - P^W &= P_{cNW}(S_W) \\ P^G - P^N &= P_{cGN}(S_T)\end{aligned}$$

$$\text{Commuting function: } S_W(P_{cNW})$$

$$S_T(P_{cGN})$$

(3) Relative permeability
– saturation
relationships

$$\begin{aligned}k_{rW}(S_W) \\ k_{rN}(S_W, S_T) \\ k_{rG}(S_T)\end{aligned}$$

$$S_T = S_W + S_N \text{ (total wetting phase)}$$

12 unknowns and 12 equations

Solve the system for 3 primary variables (saturation or pressures or mix)

Summary Governing Equations: Primary Variables P^W, S_W, S_G

Total flow equation in terms of P^W		
Sum the balance equations	$\varepsilon \partial S_W / \partial t + \nabla \cdot \mathbf{q}^W = Q^W$ $\varepsilon \partial S_N / \partial t + \nabla \cdot \mathbf{q}^N = Q^N$ $\varepsilon \partial S_G / \partial t + \nabla \cdot \mathbf{q}^G = Q^G$	$\nabla \cdot \mathbf{q}^T = Q^T$
	$S_W + S_N + S_G = 1$	
Write Darcy's law in terms of P^W	$\mathbf{q}^W = -\lambda^W (\nabla P^W - \rho^W \mathbf{g} \nabla D)$	$\mathbf{q}^T = \mathbf{q}^W + \mathbf{q}^N + \mathbf{q}^G$ $\mathbf{q}^W = -\lambda^W (\nabla P^W - \rho^W \mathbf{g} \nabla z)$ $\mathbf{q}^N = -\lambda^N (\nabla (P^W + P_{cNW}) - \rho^N \mathbf{g} \nabla z)$ $\mathbf{q}^G = -\lambda^G (\nabla (P^W + P_{cNW} + P_{cGN}) - \rho^G \mathbf{g} \nabla z)$
	$\mathbf{q}^N = -\lambda^N (\nabla P^N - \rho^N \mathbf{g} \nabla D)$	
	$\mathbf{q}^G = -\lambda^G (\nabla P^G - \rho^G \mathbf{g} \nabla D)$	
	$P^N - P^W = P_{cNW} (S_W)$ $P^G - P^N = P_{cGN} (S_T)$	
	$k_{rW} (S_W)$ $k_{rN} (S_W, S_T)$ $k_{rG} (S_T)$	$\lambda^\alpha = k k_{r\alpha} / \mu^\alpha$ (phase mobility)

Note: choose P^W because for problems involving near-surface granular soils which are partially water-saturated, water is in general continuous throughout the domain.

Summary Governing Equations: Primary Variables P^W, S_W, S_G

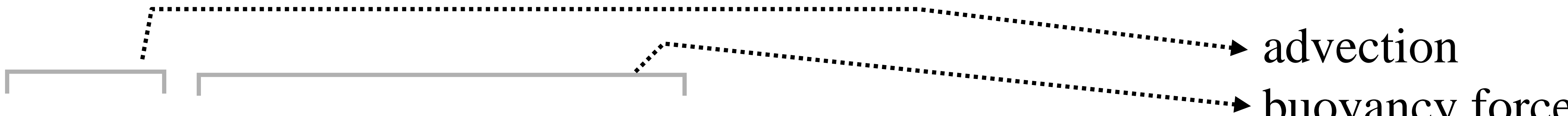
Elliptic Total Flow Equation	$\nabla \cdot \mathbf{q}^T = Q^T$	$\mathbf{q}^T = \mathbf{q}^W + \mathbf{q}^N + \mathbf{q}^G$ $\mathbf{q}^W = -\lambda^W (\nabla P^W - \rho^W \mathbf{g} \nabla z)$ $\mathbf{q}^N = -\lambda^N (\nabla (P^W + P_{cNW}) - \rho^N \mathbf{g} \nabla z)$ $\mathbf{q}^G = -\lambda^G (\nabla (P^W + P_{cNW} + P_{cGN}) - \rho^G \mathbf{g} \nabla z)$ $\lambda^\alpha = k k_{r\alpha} / \mu^\alpha \text{ (phase mobility)}$
<p>Saturation Transport Equations</p> <p>Fractional flow form (write in terms of total flow)</p>	$\varepsilon \partial S_W / \partial t + \nabla \cdot \mathbf{q}^W = Q^W$ $\varepsilon \partial S_G / \partial t + \nabla \cdot \mathbf{q}^G = Q^G$	$\mathbf{q}^W = \mathbf{f}^W \mathbf{q}^T + \mathbf{f}^W \{ \lambda^N [\nabla P_{cNW} + (\rho^W - \rho^N) \mathbf{g} \nabla z] + \lambda^G [\nabla (P_{cNW} + P_{cGN}) + (\rho^W - \rho^G) \mathbf{g} \nabla z] \}$ $\mathbf{q}^G = \mathbf{f}^G \mathbf{q}^T + \mathbf{f}^G \{ \lambda^N [\nabla P_{cGN} + (\rho^N - \rho^G) \mathbf{g} \nabla z] - \lambda^W [\nabla (P_{cNW} + P_{cGN}) + (\rho^W - \rho^G) \mathbf{g} \nabla z] \}$ $\mathbf{f}^\alpha = \lambda^\alpha / (\lambda^N + \lambda^W + \lambda^G) \quad \text{fractional flow}$

Fractional flow form of the S_w equation w/ no source/sink
(example for nonlinear advection-diffusion equations)

Water balance for a water-NAPL system

$$\partial S_w / \partial t + \mathbf{q}^w \cdot \nabla S_w - \nabla \cdot (\mathbf{h}^w \cdot \nabla S_w) = 0$$

where:



$$\mathbf{q}^w = [(\mathbf{f}^w)' \mathbf{q}^T + (\mathbf{f}^w \lambda^N)' (\rho^N - \rho^w) \mathbf{g} \nabla \mathbf{D}]$$

water wave speed

$$\mathbf{h}^w = \mathbf{f}^w \lambda^N (\mathbf{P}_{NW})'$$

capillary diffusion

$$\mathbf{f}^w = \lambda^w / (\lambda^N + \lambda^w)$$

fractional flow of water

$$\mathbf{q}^T = \mathbf{q}^w + \mathbf{q}^N$$

total fluid flow

$$(\bullet)' = d(\bullet) / d S_w$$

derivative notation

PECLET and COURANT CRITERIA

Local Peclet number: $Pe = \mathbf{q}^w \Delta s / \mathbf{h}^w$

Local Courant number: $Co = \mathbf{q}^w \Delta t / \Delta s$

Periodic injection of DNAPL

$$\partial S_w / \partial t + \mathbf{q}^w \cdot \nabla S_w - \nabla \cdot (\mathbf{h}^w \cdot \nabla S_w) = 0$$

$$\mathbf{q}^w = [(\mathbf{f}^w)' \mathbf{q}^T + (\mathbf{f}^w \lambda^N)' (\rho^N - \rho^w) \mathbf{g} \nabla D] \quad \text{water wave speed}$$

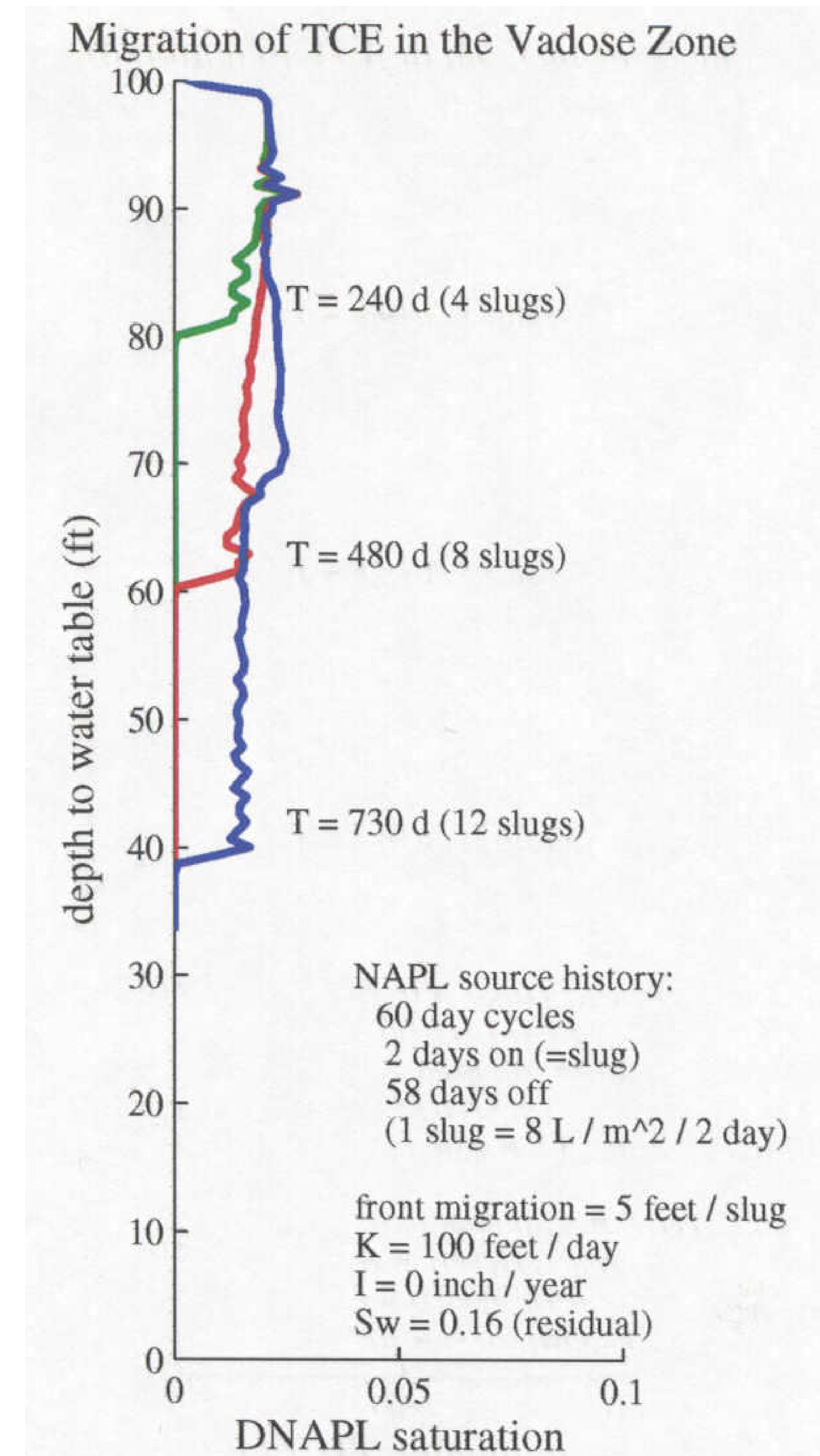
$$\mathbf{h}^w = \mathbf{f}^w \lambda^N (P_{NW})' \quad \text{capillary diffusion}$$

$$\mathbf{f}^w = \lambda^w / (\lambda^N + \lambda^w) \quad \text{fractional flow of water}$$

$$\mathbf{q}^T = \mathbf{q}^w + \mathbf{q}^w \quad \text{total fluid flow}$$

$$(\bullet)' = d(\bullet) / d S_w \quad \text{derivative notation}$$

Note front speed and front shape, they are constant



Sequential solution of the total flow formulation

STEP 1

Fix S_W, S_G and solve for P^W (= linear, elliptic equation)
Then compute \mathbf{q}^T

$$\nabla \cdot \mathbf{q}^T = Q^T$$

$$\mathbf{q}^T = \mathbf{q}^W + \mathbf{q}^N + \mathbf{q}^G$$

$$\mathbf{q}^W = -\lambda^W (\nabla P^W - \rho^W \mathbf{g} \nabla z)$$

$$\mathbf{q}^N = -\lambda^N (\nabla (P^W + P_{cNW}) - \rho^N \mathbf{g} \nabla z)$$

$$\mathbf{q}^G = -\lambda^G (\nabla (P^W + P_{cNW} + P_{cGN}) - \rho^G \mathbf{g} \nabla z)$$

$$\lambda^\alpha = k k_{r\alpha} / \mu^\alpha \text{ (phase mobility)}$$

STEP 2

Given \mathbf{q}^T , sequentially solve the water and gas equations, iterating to convergence (= nonlinear, coupled, parabolic equations)

$$\varepsilon \partial S_W / \partial t + \nabla \cdot \mathbf{q}^W = Q^W$$

$$\mathbf{q}^W = \mathbf{f}^W \mathbf{q}^T + \mathbf{f}^W \{ \lambda^N [\nabla P_{cNW} + (\rho^W - \rho^N) \mathbf{g} \nabla z] + \lambda^G [\nabla (P_{cNW} + P_{cGN}) + (\rho^W - \rho^G) \mathbf{g} \nabla z] \}$$

$$\varepsilon \partial S_G / \partial t + \nabla \cdot \mathbf{q}^G = Q^G$$

$$\mathbf{q}^G = \mathbf{f}^G \mathbf{q}^T + \mathbf{f}^G \{ \lambda^N [\nabla P_{cGN} + (\rho^N - \rho^G) \mathbf{g} \nabla z] - \lambda^W [\nabla (P_{cNW} + P_{cGN}) + (\rho^W - \rho^G) \mathbf{g} \nabla z] \}$$

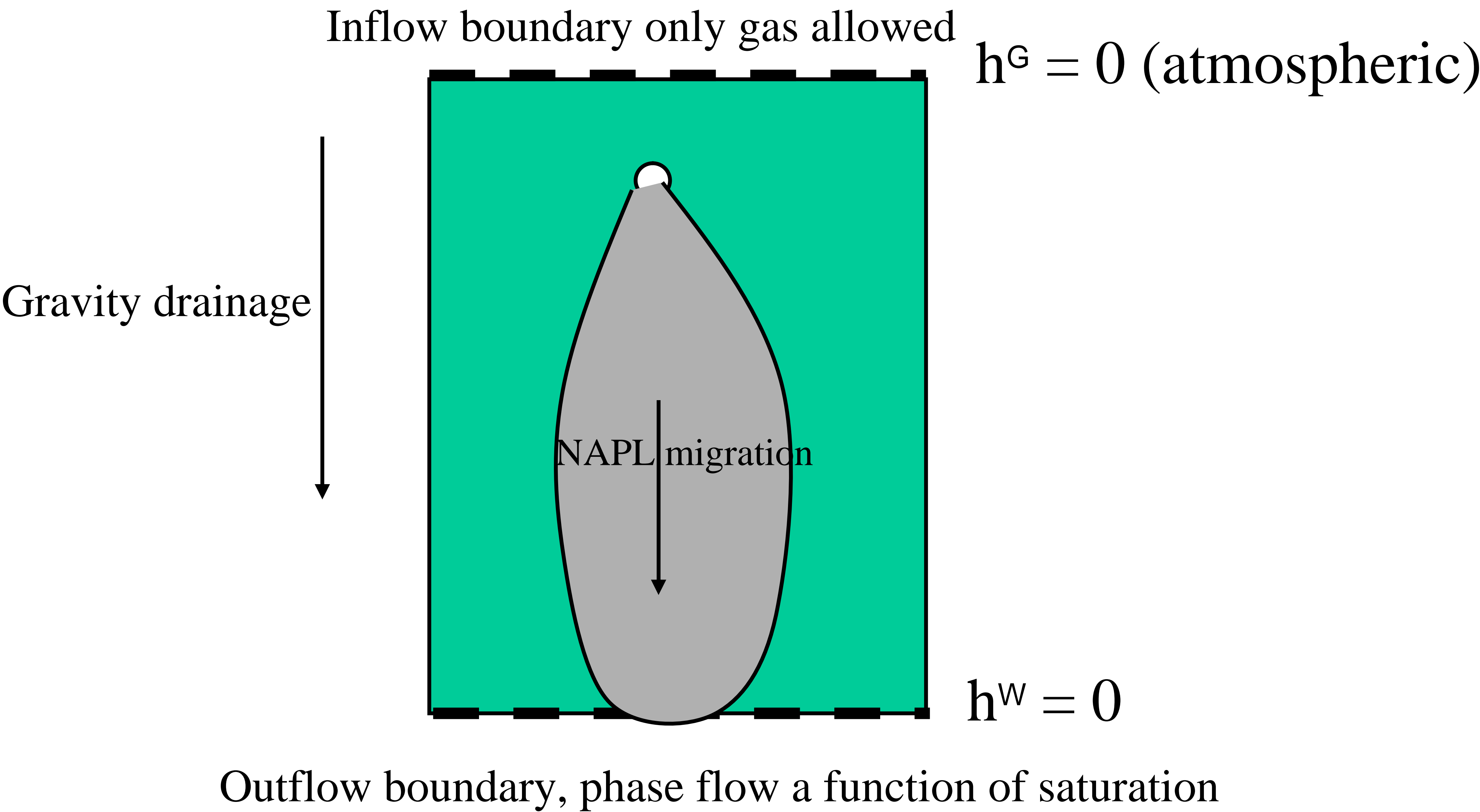
$$\mathbf{f}^\alpha = \lambda^\alpha / (\lambda^N + \lambda^W + \lambda^G) \quad \text{fractional flow}$$

Flow Boundary Conditions

case	boundary open (o) or closed (x) to inflow of a phase			variables specified	condition for the primary variable 1 = Dirichlet 2 = Neuman (L = linear, NL = nonlinear)			comment
	Water	NAPL	Gas		P ^W	S _w	S _g	
1	x	x	x		2(L)	2(NL)	2(NL)	the default condition
2	x	x	o	P ^G	2(L)	2(NL)	2(NL)	replace with source term
3	x	o	x	P ^N	2(L)	2(NL)	2(NL)	replace with source term
4	o	x	x	P ^W	1(L)	2(NL)	2(NL)	
5	o	o	o	P ^W , S _w , S _G	1(L)	1(L)	1(L)	

If outflow conditions prevail, preserve pressure but set flux based on fractional flow

$$Q^\alpha = \mathbf{f}^\alpha \mathbf{q}^T, \quad \mathbf{f}^\alpha = \lambda^\alpha / (\lambda^N + \lambda^W + \lambda^G)$$



External Flux Conditions (Wells)

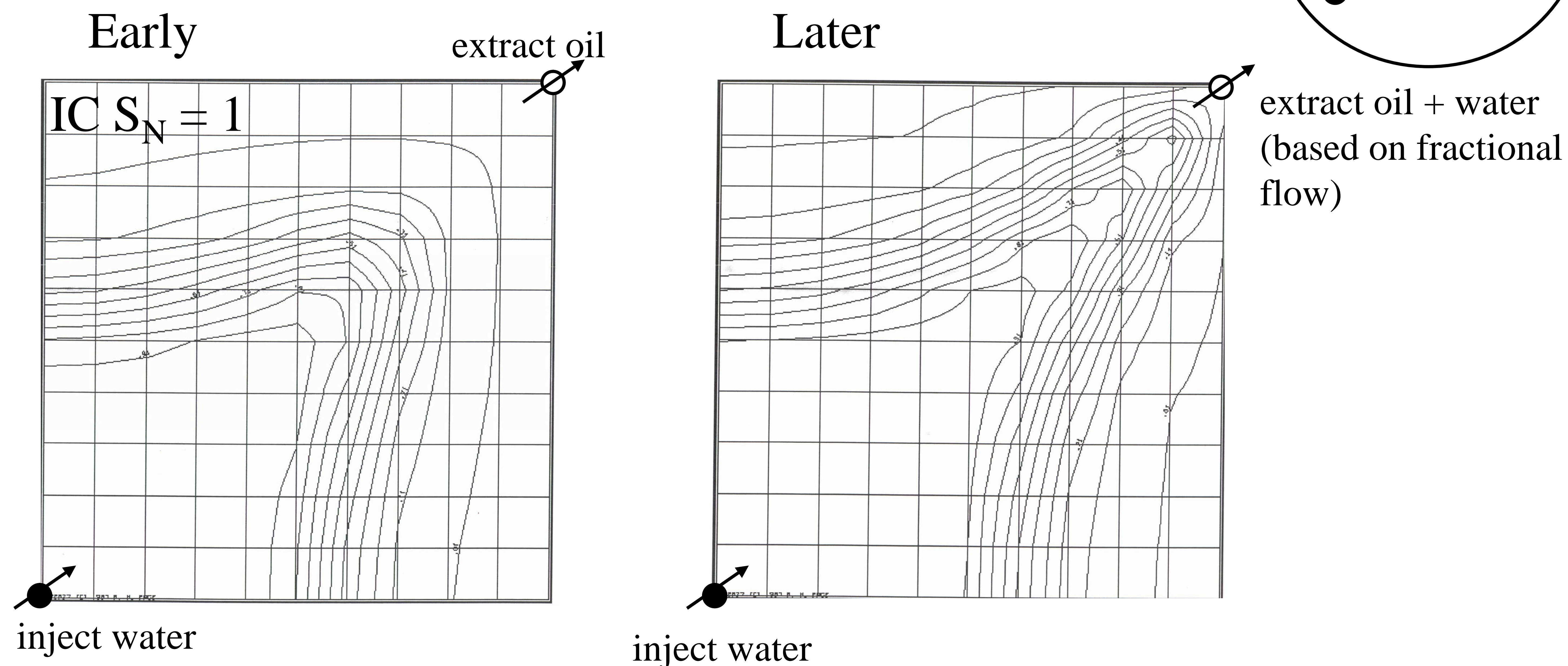
Specify flux rate

If injection then specify fractional flow (e.g., all water, $f^W = 1$)

If extraction fractional flow a function of saturation:

$$Q^\alpha = f^\alpha q^T, \quad f^\alpha = \lambda^\alpha / (\lambda^N + \lambda^W + \lambda^G)$$

Consider the classic five spot pattern in oil reservoir simulation



Initial Conditions for Flow

P^W doesn't need an initial condition

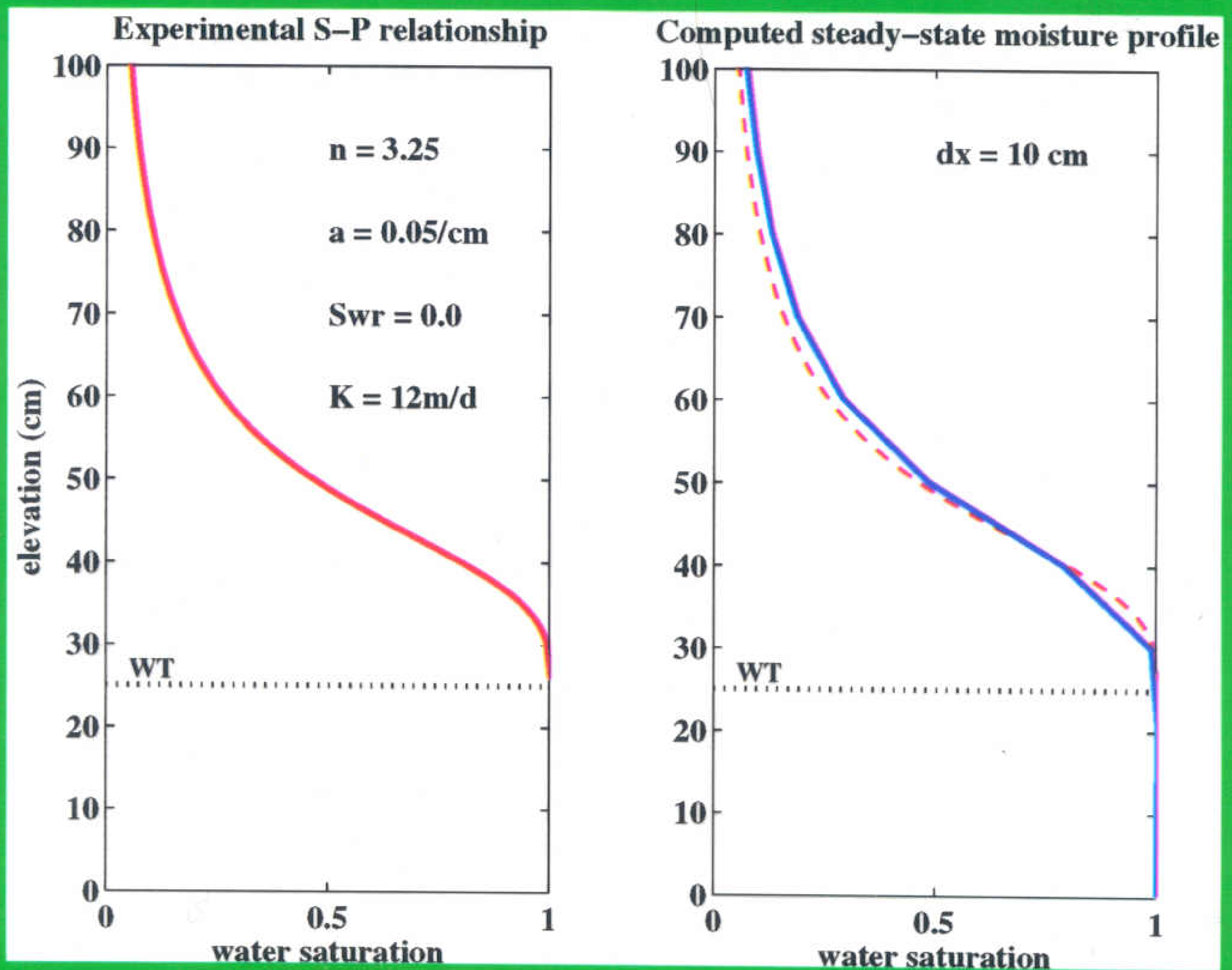
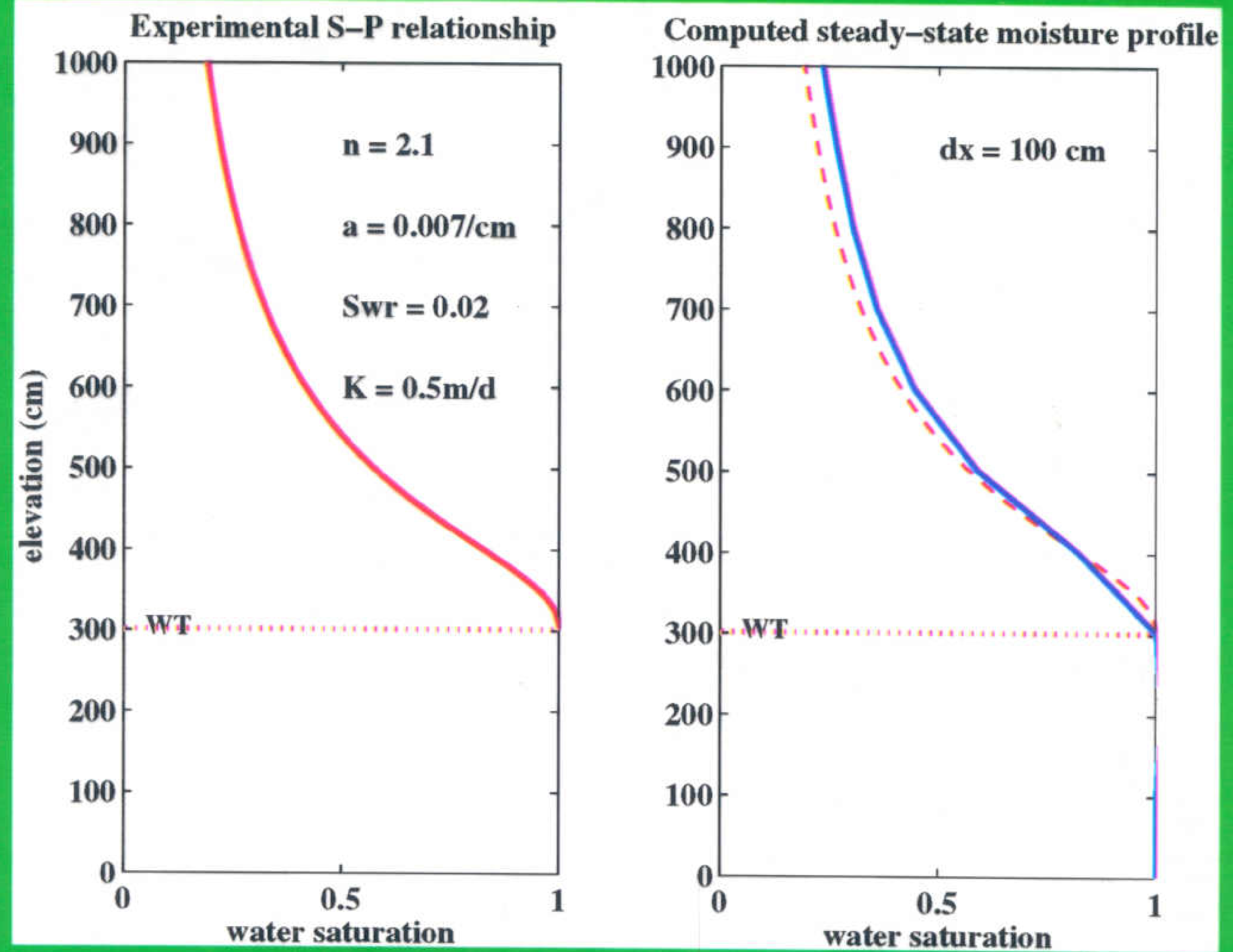
S_W, S_G need an IC

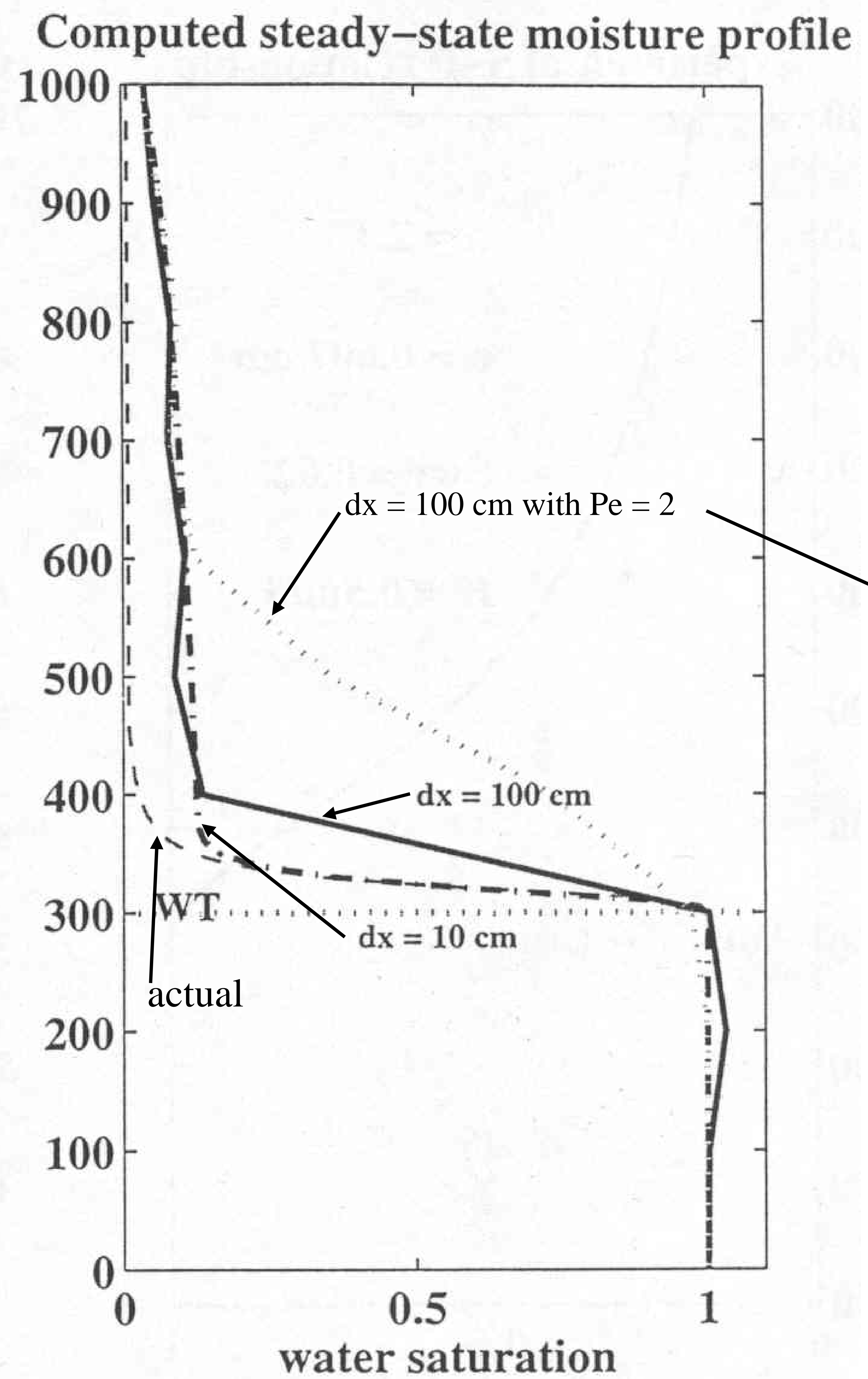
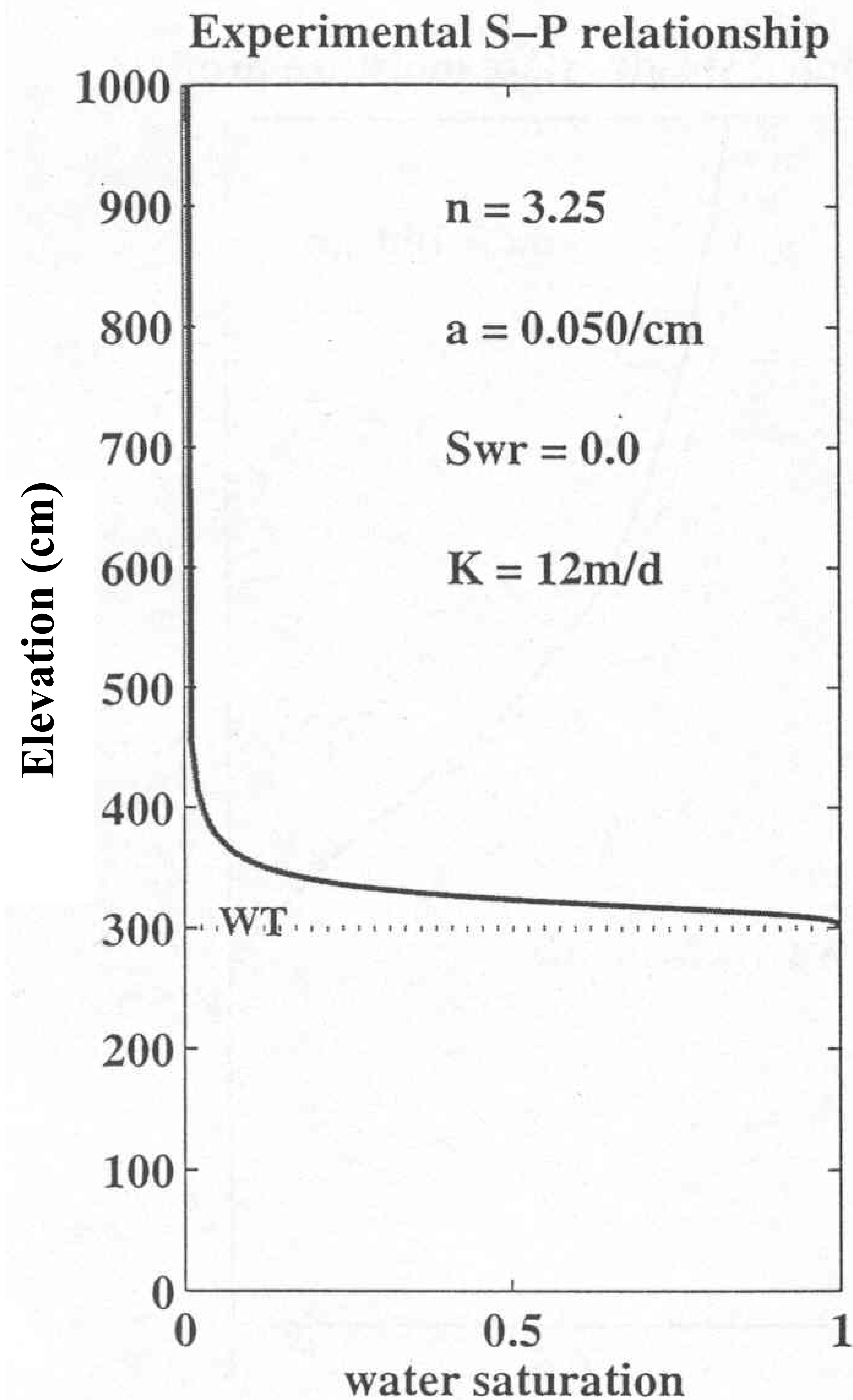
Summary: any phase configuration yielding $S_W + S_N + S_G = 1$ is admissible

Model Validation and Verification

test	purpose
Convergence in time and space	self consistency
mass balance	self consistency
comparison to analytical solutions	self consistency
comparison to experimental results	verify physics

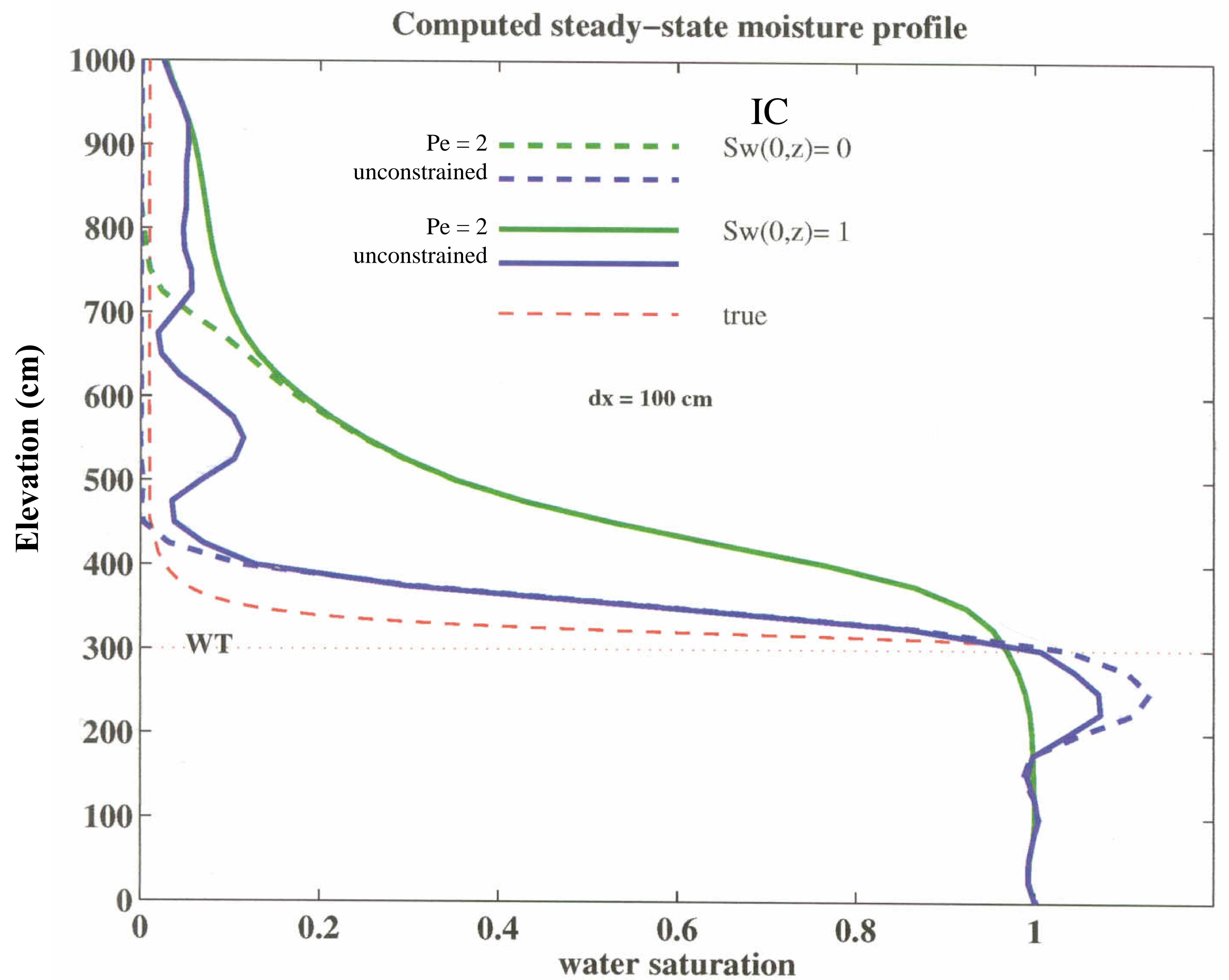
Appropriate grid scale is a function of the physical parameters



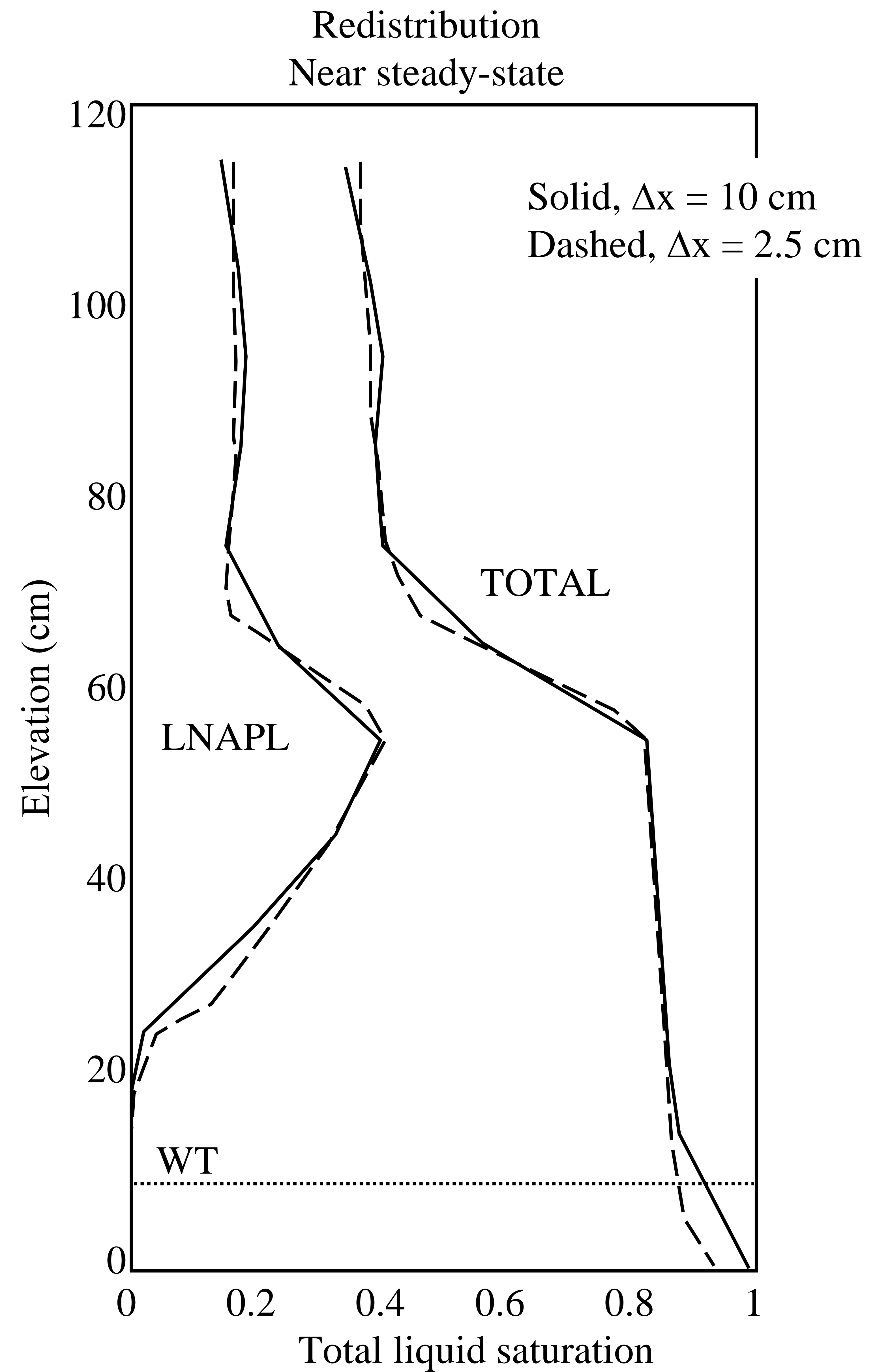
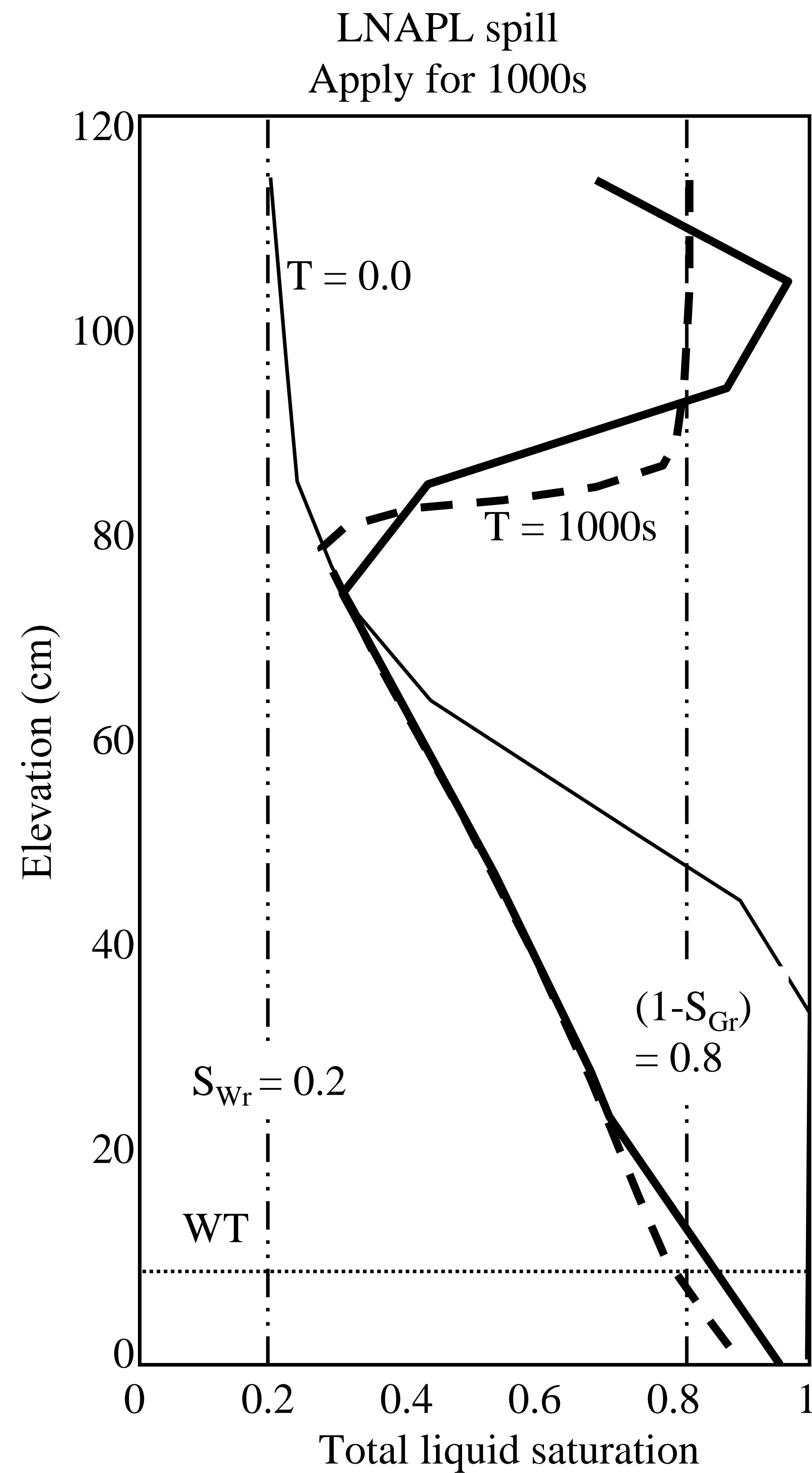


Peclet constraint = adjust capillary diffusion such that the solution and the grid are compatible

$$Pe = \mathbf{q}^W \Delta s / \mathbf{h}^W$$



The simulator can handle some oscillations



EXAMPLE – 1-D profiles: DNAPL imbibition (1D_NAPL.xls)

k-S-P model (van Genuchten)

$\alpha_d = 0.1 / \text{cm}, \alpha_d = 0.2 / \text{cm}$

$n = 6$

$S_{Wr} = 0.2, S_{Nr} = 0.3$

$\Delta x = 5 \text{ cm}$

Static water $H_W = 0$

DNAPL sources
 $0.02 \text{ cm}^3/\text{s}$

IC: $S_w = 1.0$
 $k = 5.0 \text{ e} - 7 \text{ cm}^2$

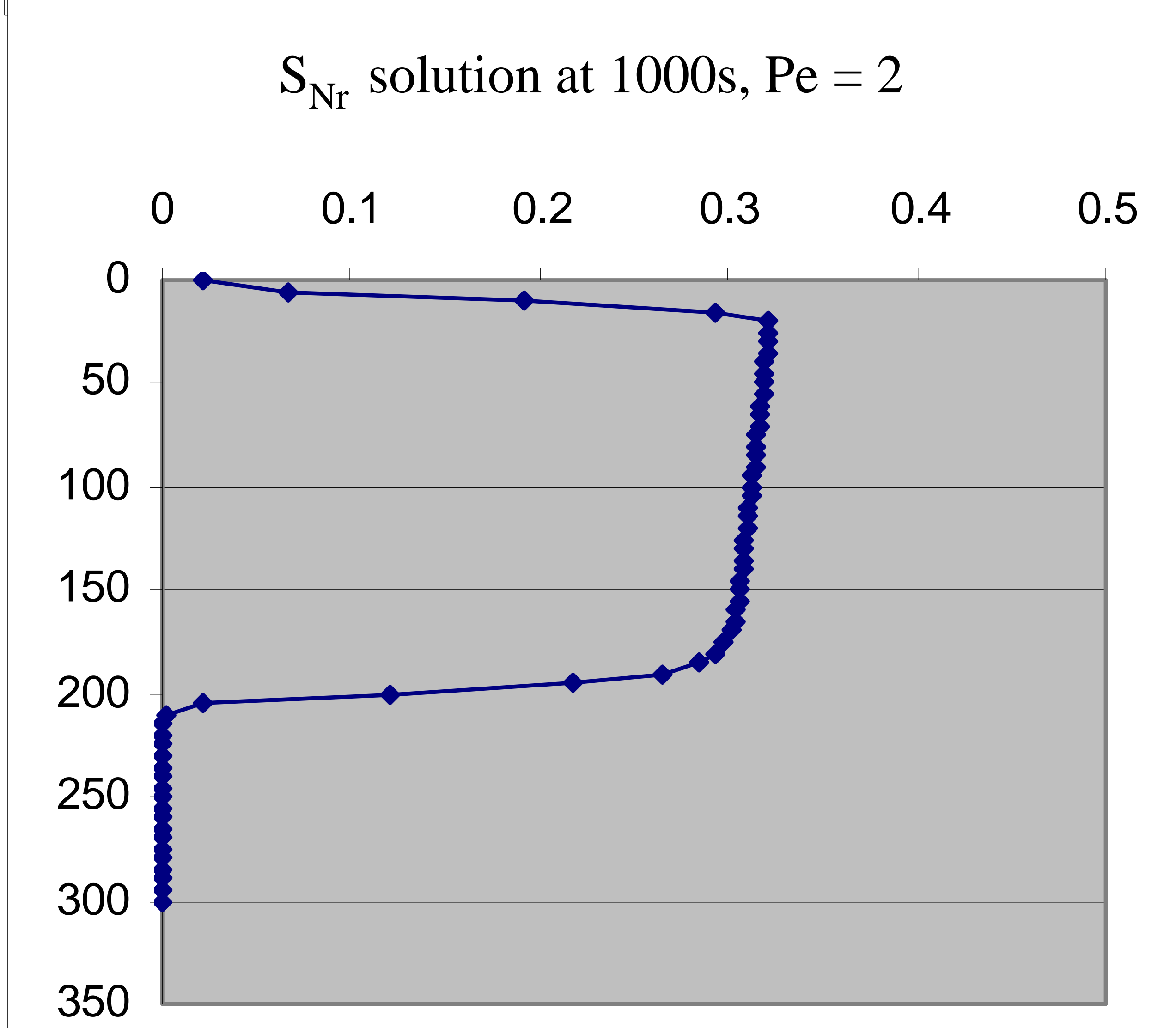
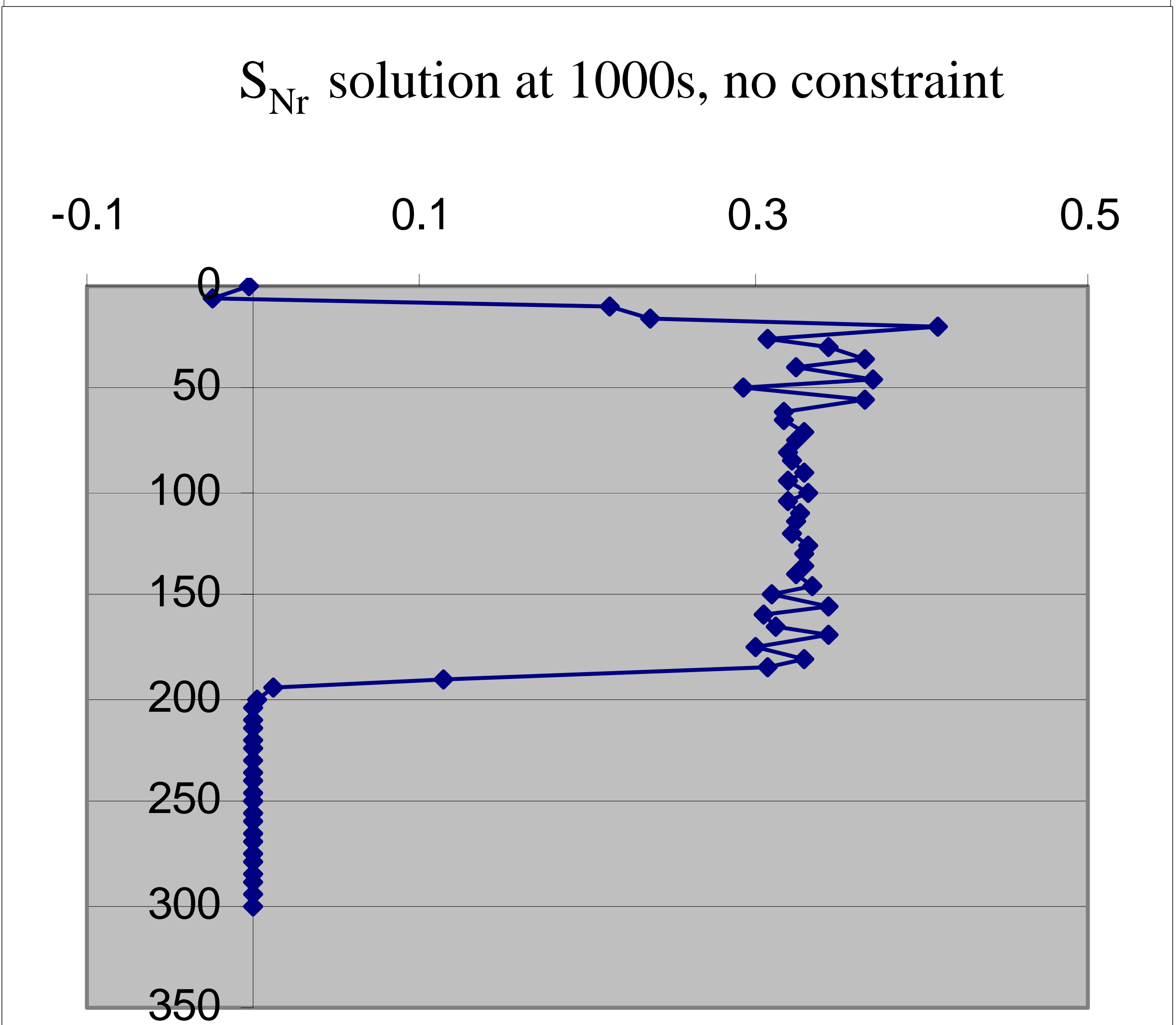
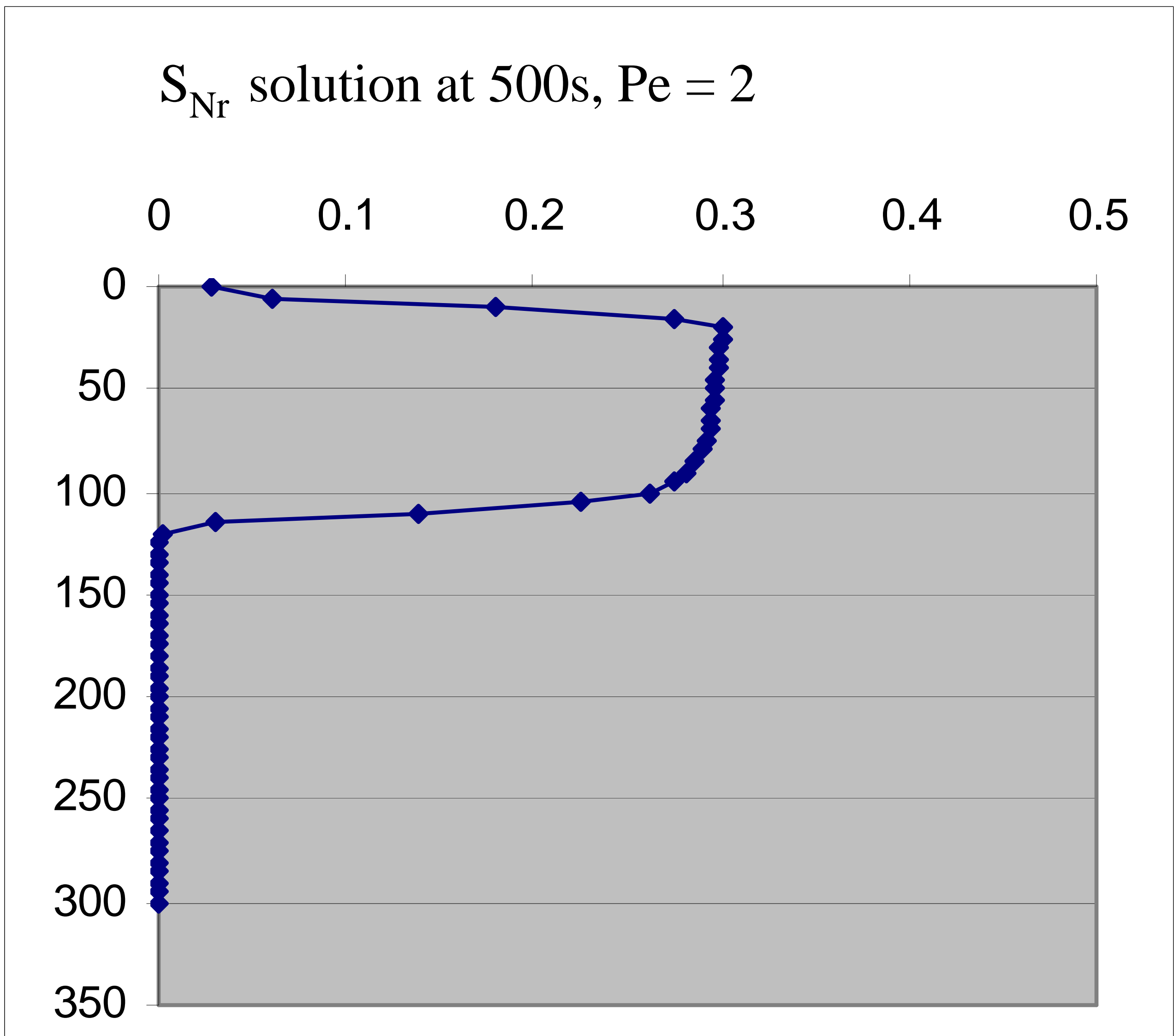
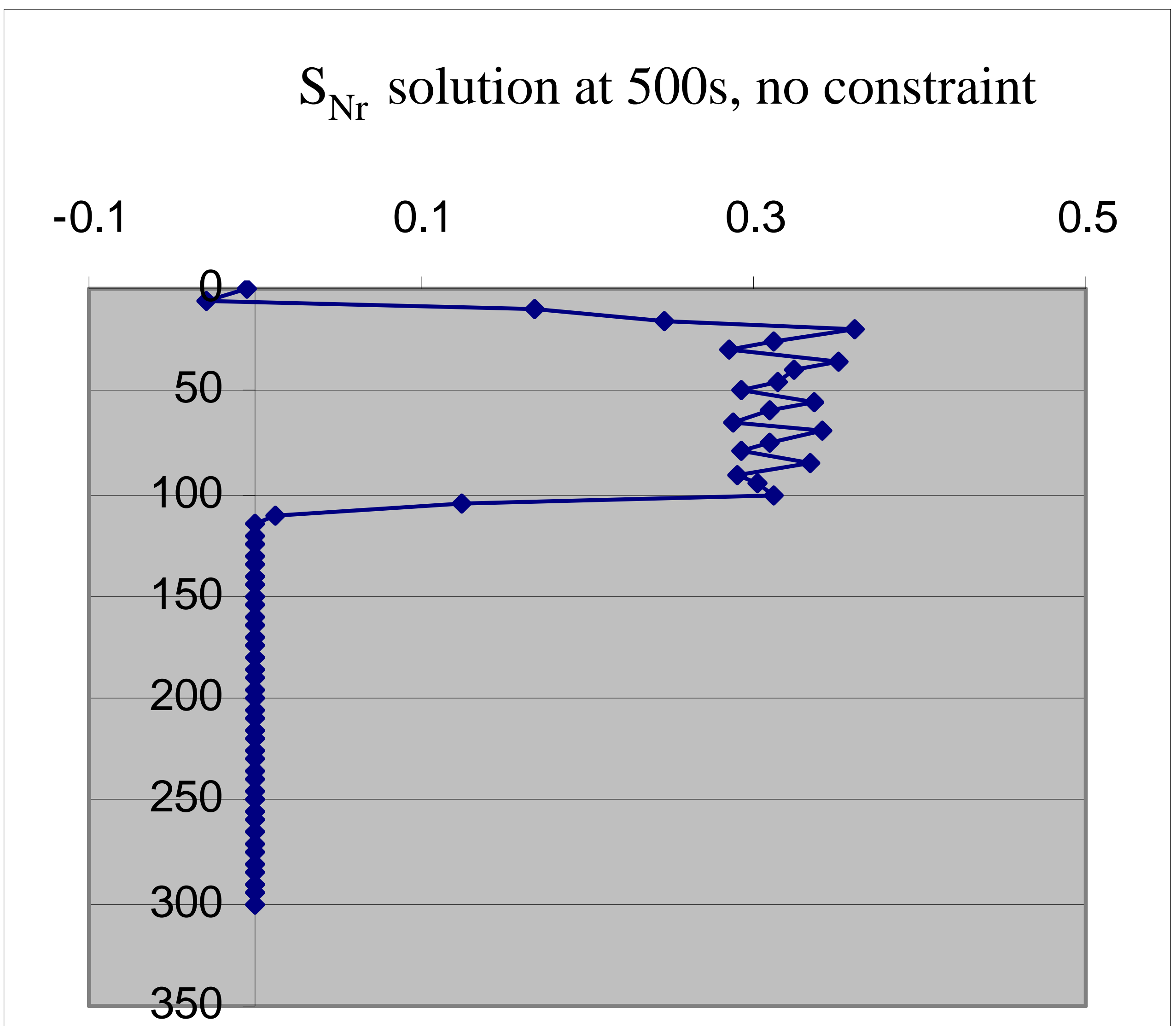
no flow

no flow

300 cm

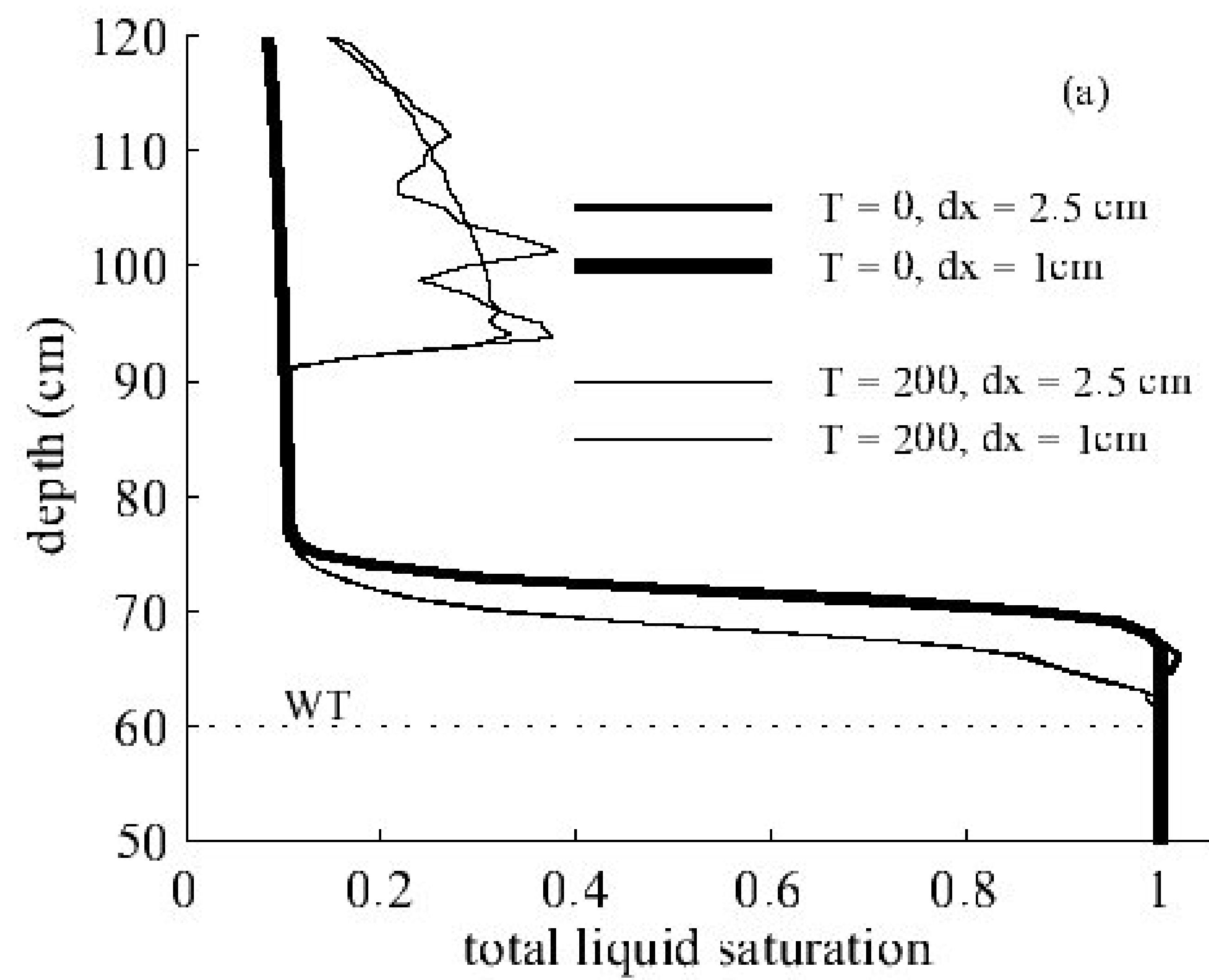
$H_W = 30 \text{ cm}$

2 cm

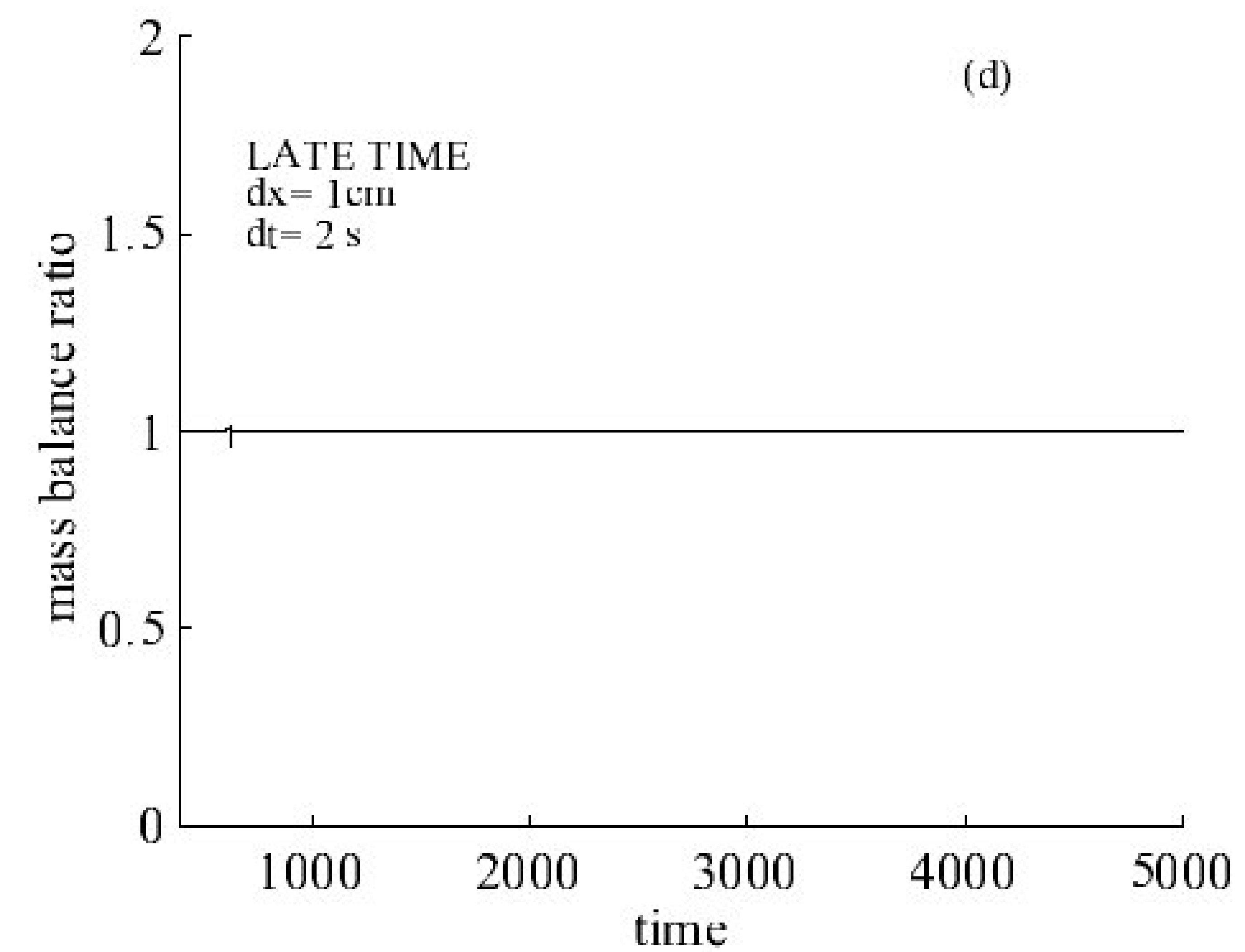
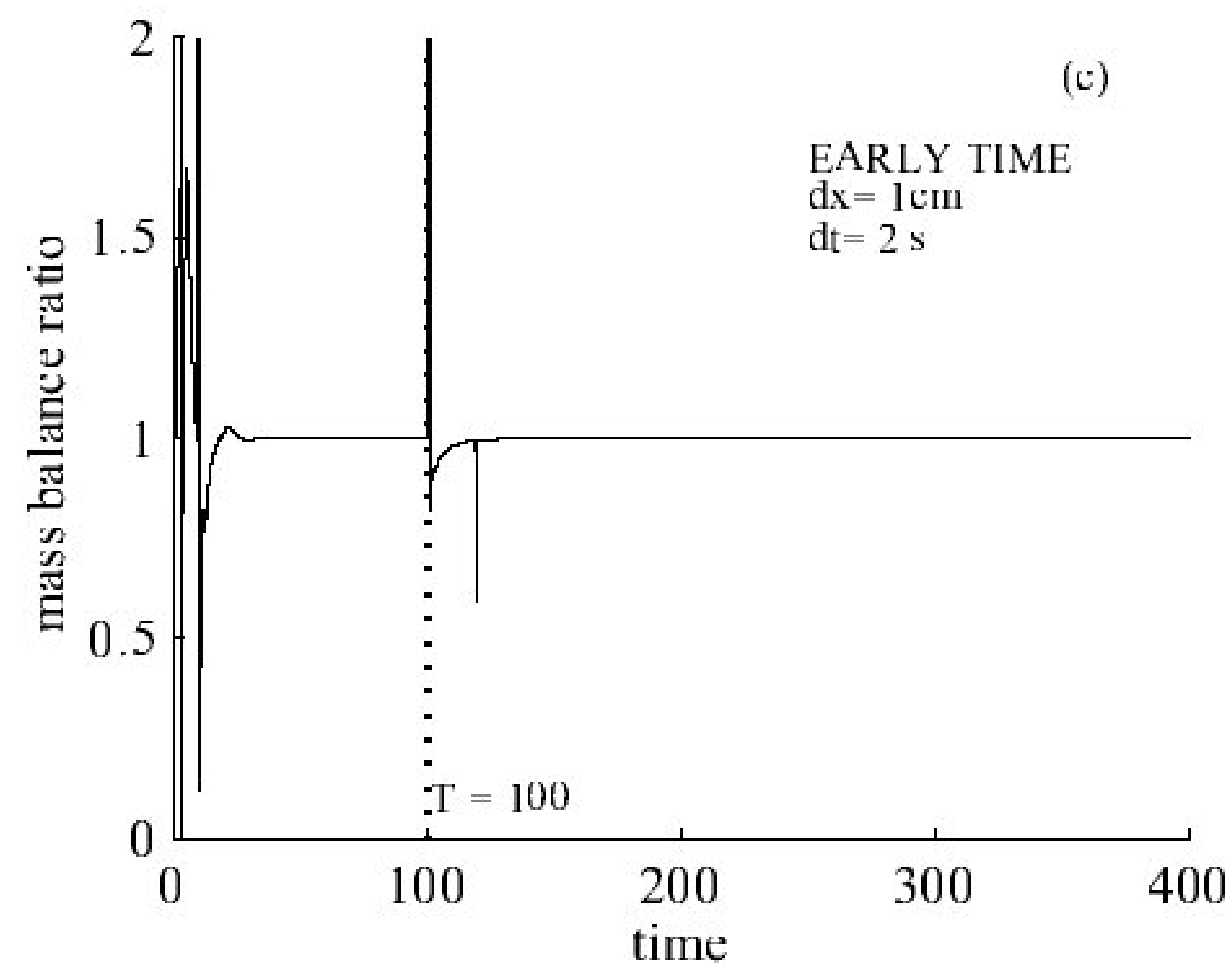
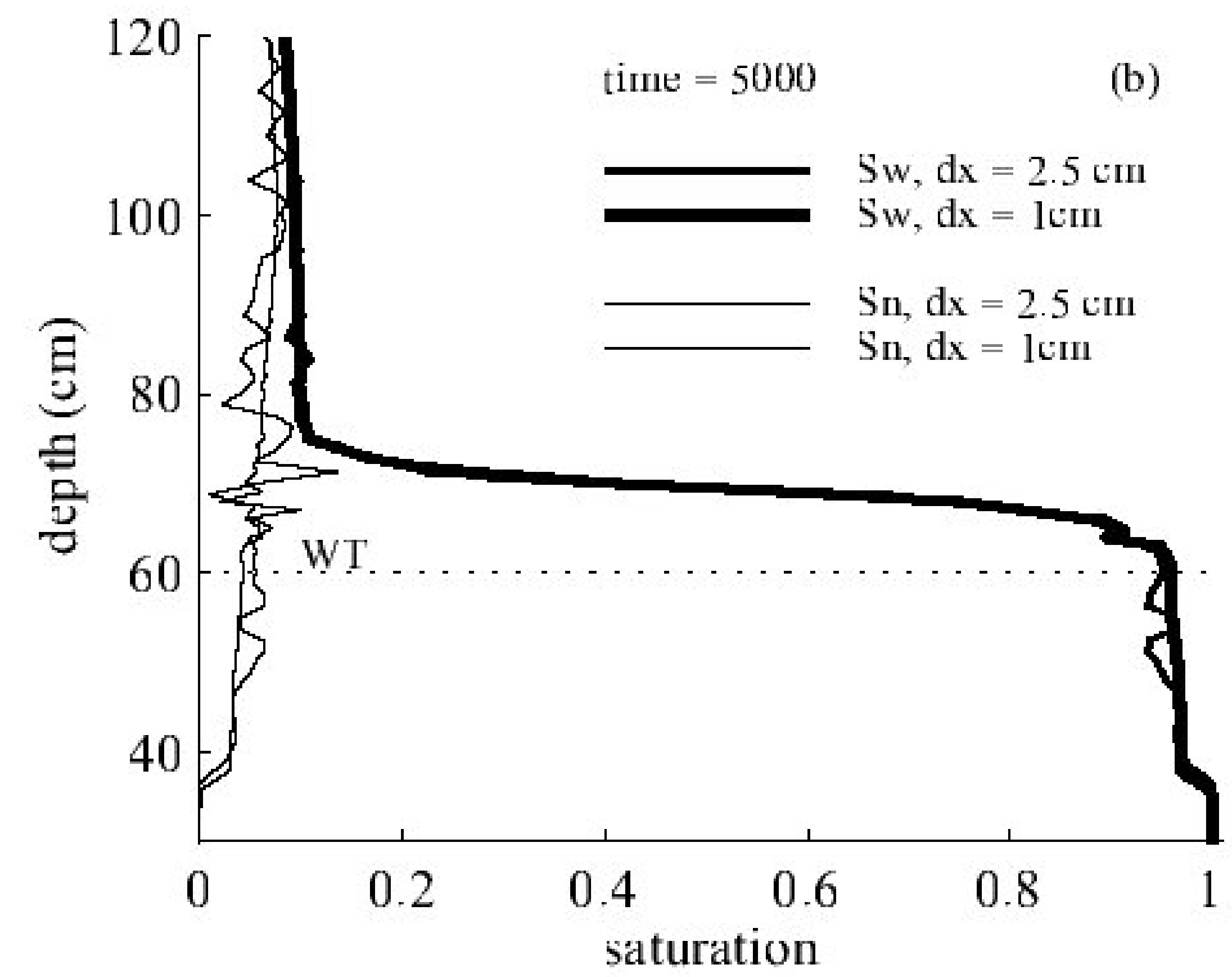


Convergence and mass balance.

3-phase DNAPL flood

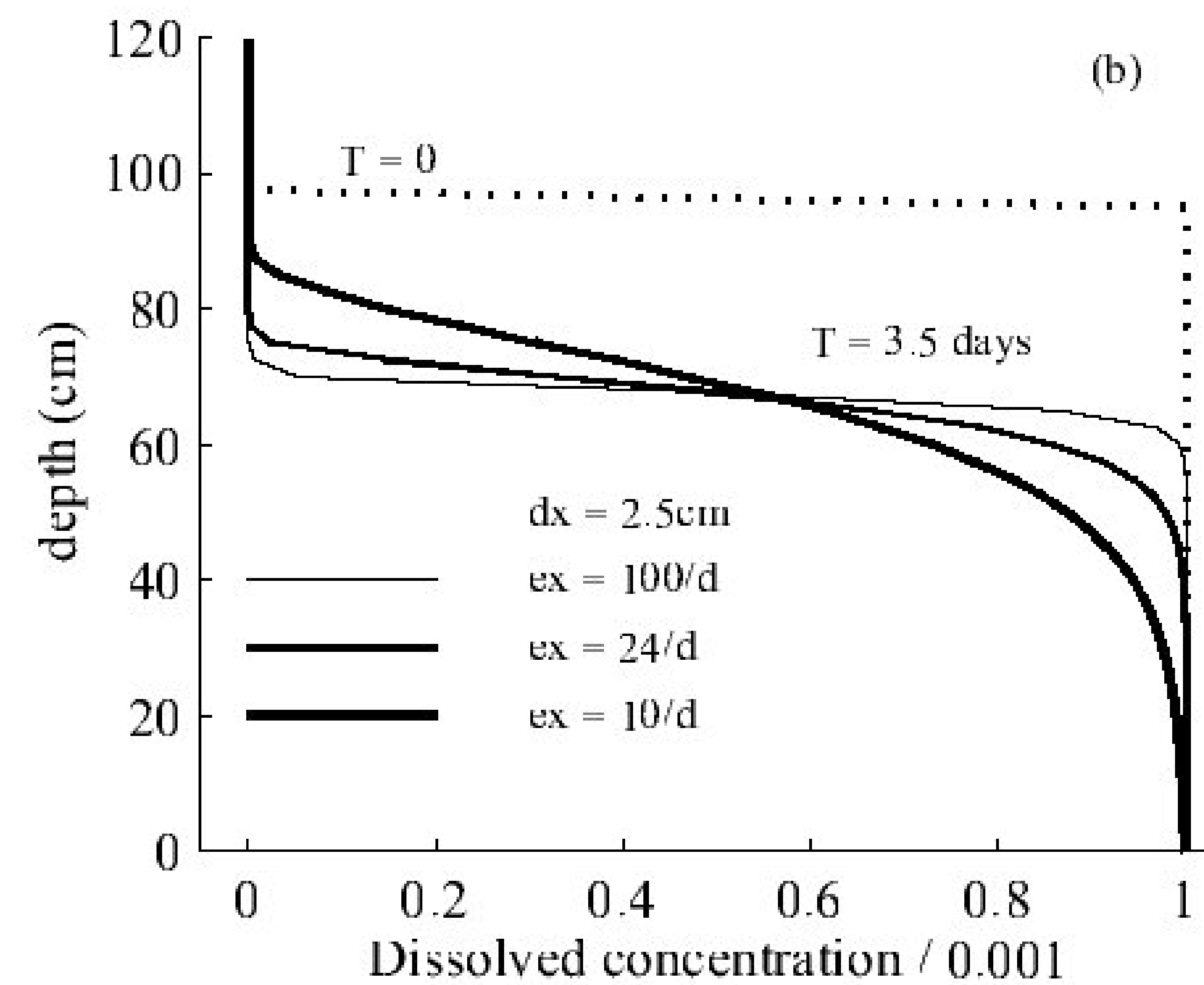
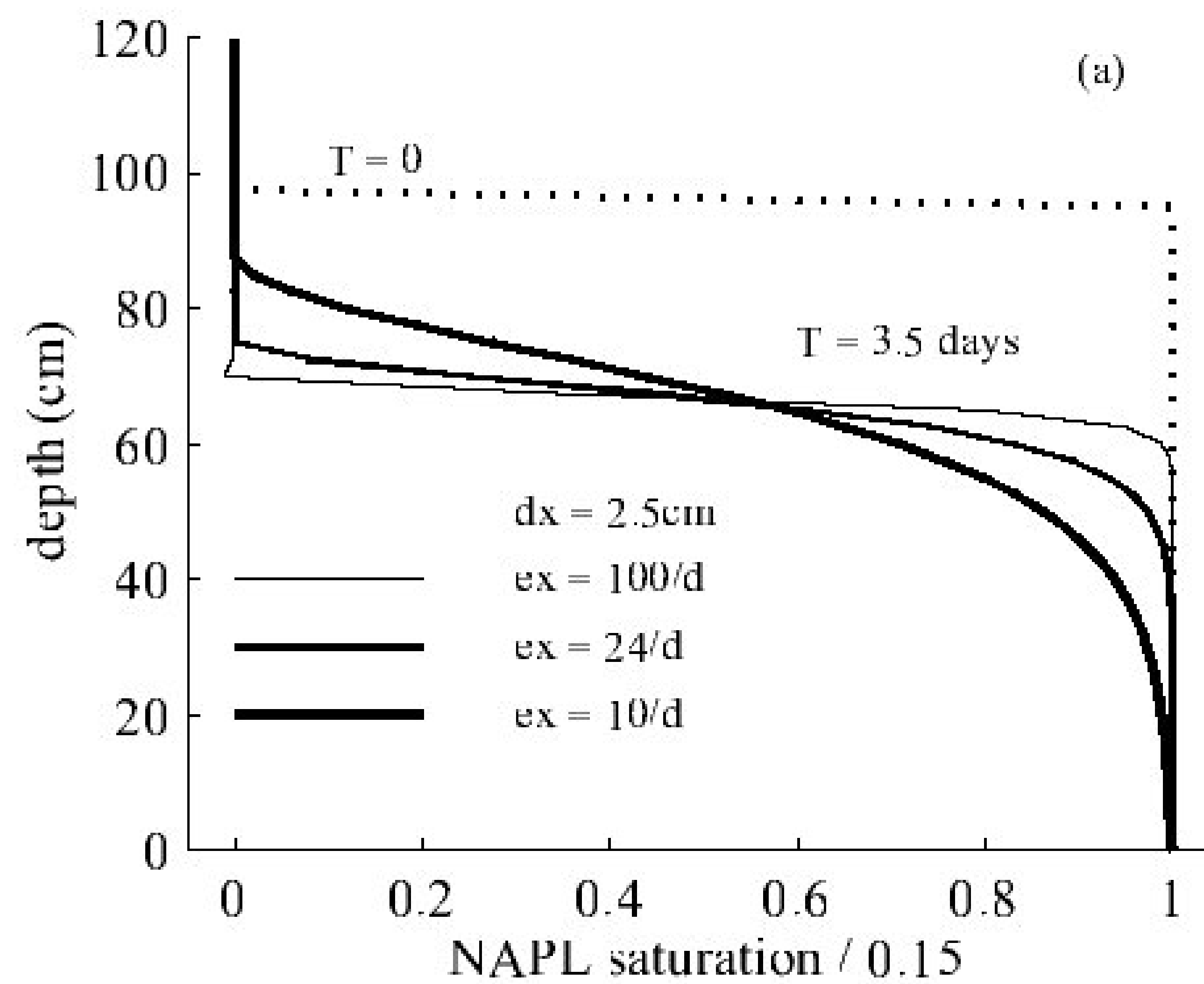


DNAPL redistribution

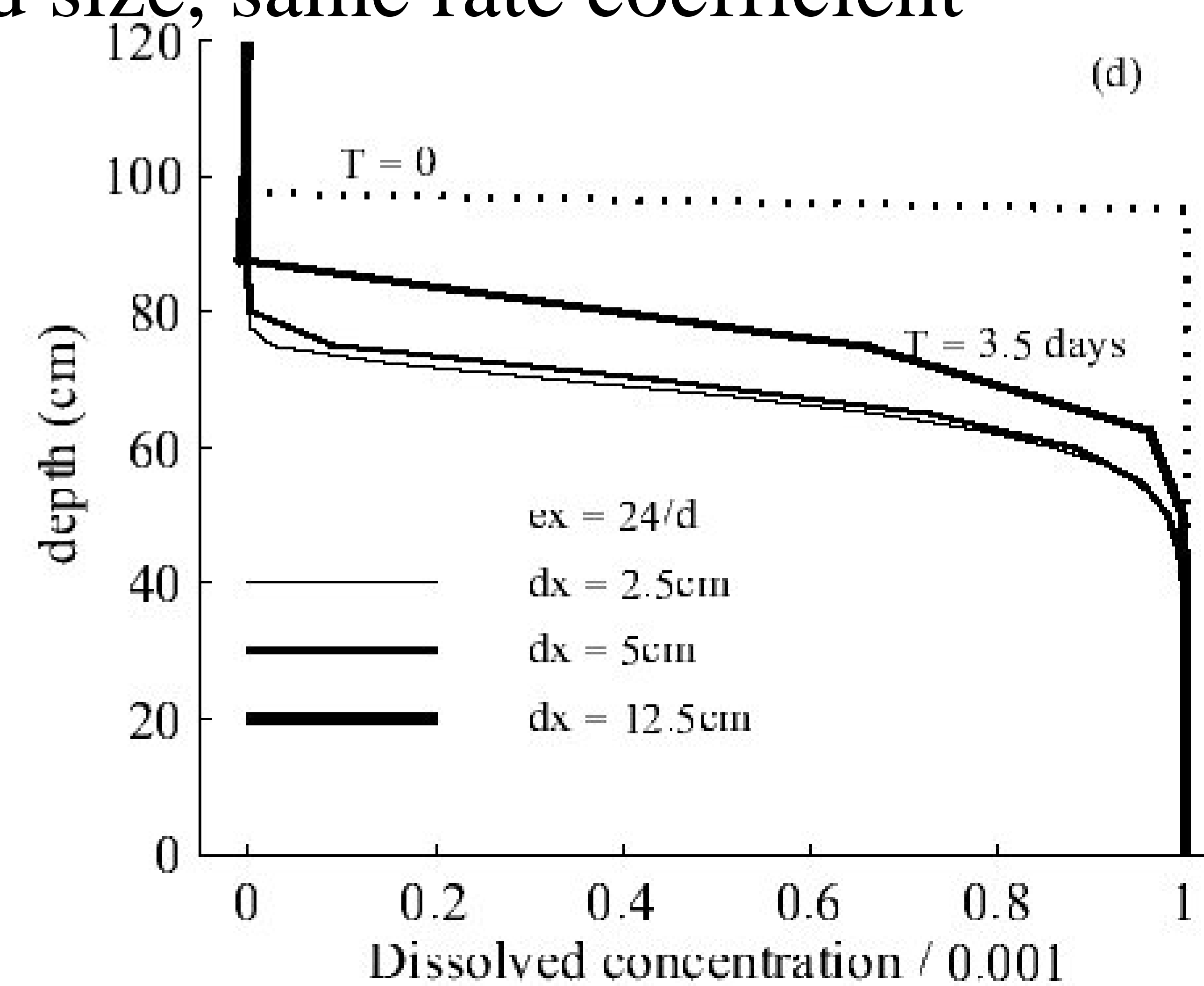
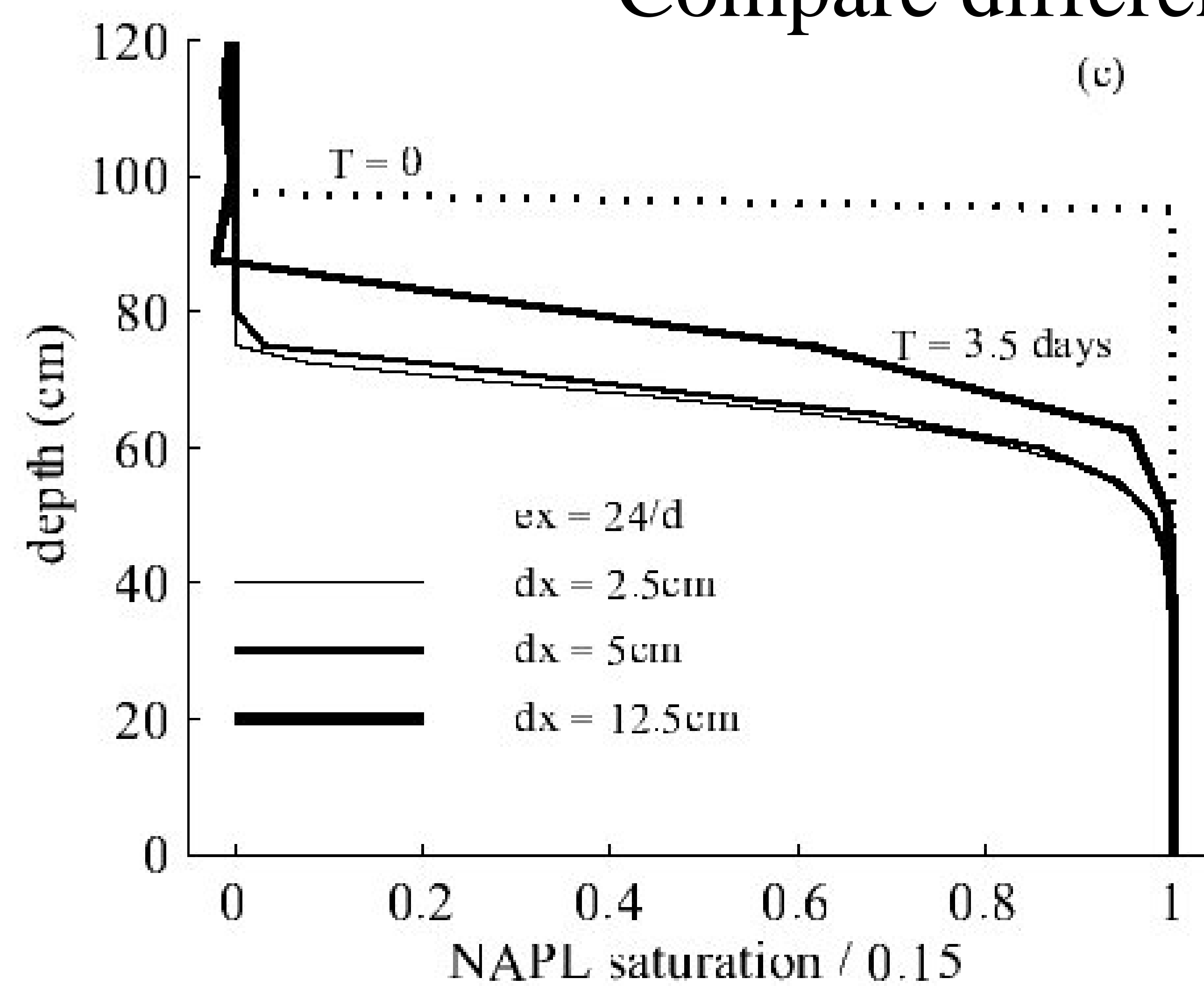


DNAPL dissolution mass exchange – spatial convergence and grid compatibility.

Compare different rates, constant grid size



Compare different grid size, same rate coefficient



Summary of Simulator Capabilities - Numerics

- Code written in FORTRAN 77 (compiled using Lahey F90 and F95 and Visual FORTRAN V5)
- 2-D and 3-D versions.
- Finite element discretization with continuous velocity field
- Memory intensive, especially in 3-D. Therefore, not amenable to large 3-D field simulations.
- No upstream weighting (add diffusion explicitly using Peclet constraint).
- Sequential solution of balance equations
 - o minimize system matrix size
 - o parallel processing of transport equations (saturation and concentration)
 - o facilitate adding additional species and processes
- Flow boundary conditions
 - o specify Dirichlet data for any phase pressure or saturation
 - o specify flux of any phase

MODEL I/O Attributes

Internal input stream error checking

Unformatted input

Restart capability – read in existing solution as IC's

Change forcing on the fly – change BC's and external forcing at specified times

Automated time step control

Input using any self-consistent units (e.g., CGS).

Diagnostic tools:

- mass balance output
- time step and iteration performance (nonlinear and CG solver)
- Peclet Constraint

Pre-processing

- Excel

Visualization

- output at specified times
- formatted for GMS

Sensitive Parameters for NAPL-Site Characterization and Simulation

FLUID FLOW

- System Forcing in time and space (NAPL, rain)
- Soil Permeability (heterogeneity)
- Residual NAPL saturation

CONTAMINANT TRANSPORT AND FATE

- Moisture content in vadose zone
- organic carbon content
- Natural degradation rate
- rate-limited mass exchange (defines source mass loading)

DISCRETE REPRESENTATION

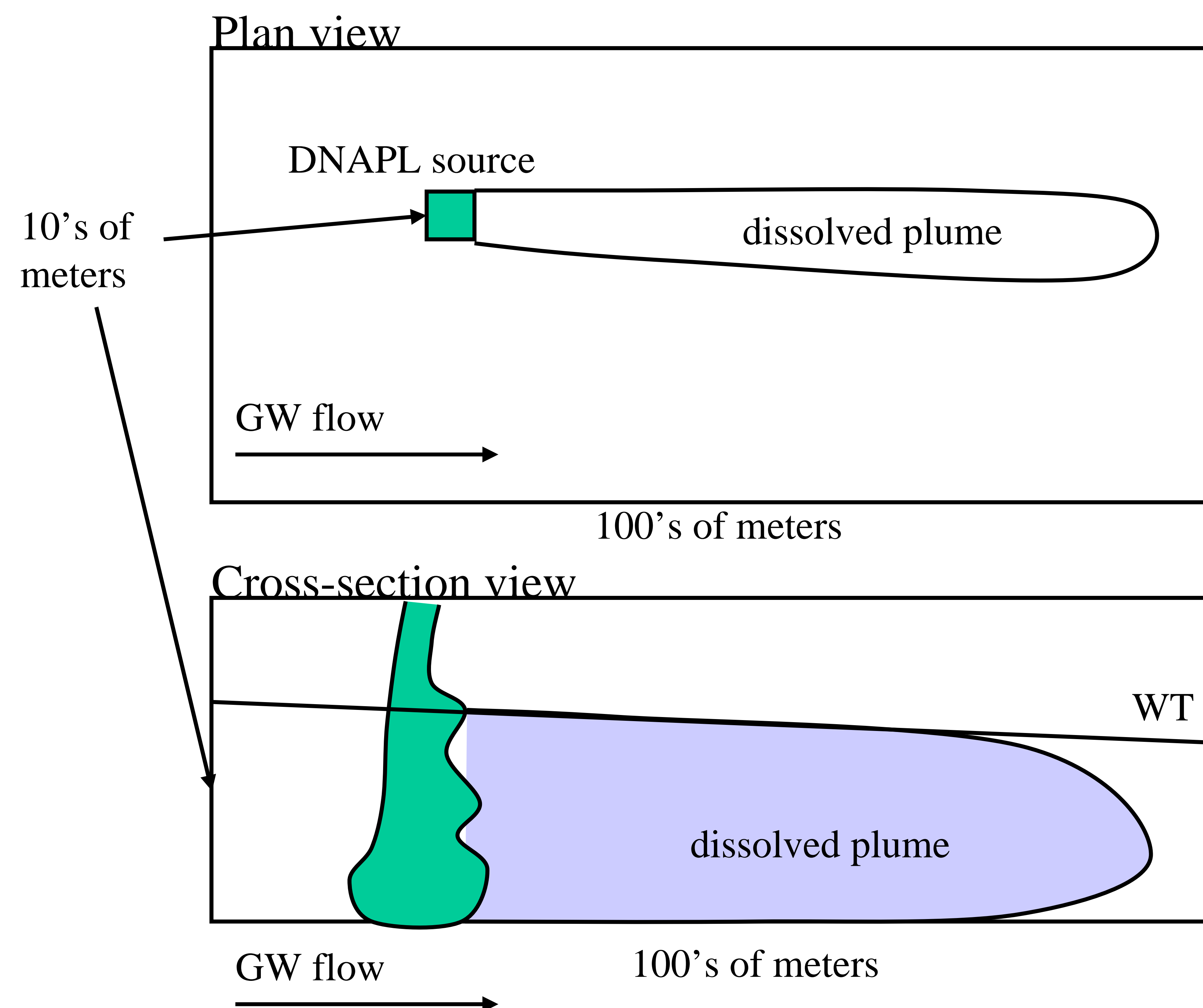
- Time step
- Space step

MODEL UTILITY

Research tool – assess conceptual/empirical models of the physics at the experimental-scale (order of meters)

Consulting Tool

- concept development: educational tool, process presentation
- Field-scale modeling



Use the NAPL Simulator to model the **source only**

Define mass flux as a function of time

Use mass flux as input to an efficient transport model (e.g., PTC, MOC3D, etc.)

MODEL LIMITATIONS

Computationally intensive:

- coupled non-linear equations
- large system matrix
- not amenable to large 3-D problems

Instabilities at the capillary fringe

- difficult to model because of poor matrix conditioning at liquid-air interface

Model improvements are ongoing.

Comparison of the Physical Attributes Describing Water-Resources and Petroleum-Reservoir NAPL Recovery applications

attribute	water-resources	petroleum-reservoir
motivation	protect human and enviro. Health	max economic recovery of hydrocarbons
scale	spatial - meters to 10s of meters	spatial - Km
	temporal - days to decades	temporal - months to years
geology	unconsolidated	consolidated sediment
	granular to clay, organic matter	sandstone, limestone
	primary porosity	secondary porosity
pressure	atmospheric	high pressure
	fluid properties not strong functions of pressure	fluid properties are strong functions of pressure
fluid types	gas = air	gas = methane
	water = relatively pure	water = connate, saline
	NAPL = BTEX, solvents, LNAPL, DNAPL	NAPL = raw petro. liq., high viscosity, LNAPL
system forcing	precipitation	initially = difference between atm. and res. Pressure
	hydraulic gradient	wells
	wells	gravity drainage
	NAPL source history	expansion effects due to pressure Release
	gravity	
	capillarity	
NAPL recovery techniques	dissolved plume pump-and-treat	primary = pump oil under natural gradients
	pump LNAPL product using gravity drainage	secondary = water flood displacement
	source remediation: SVE, surfactant, co-solvent, steam flush, bio-remediation, reactive filter	tertiary = remove residual by surfactant, cosolvent, steam flush