Detailed modeling of soil vapor extraction systems

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ABSTRACT: This paper presents results of a numerical investigation of soil vapor extraction systems (SVE) at the laboratory scale. Modeling of transport, dispersion and interfacial transfers is done using effective parameters of the local volume averaging theory. The main focus is on the detailed description of the physical and chemical processes that govern the kinetics of mass and energy transfer across the solid, fluid and gaseous phases. Simulations are carried out in two dimensions. The system of partial differential equations is discretized by a finite volume method and an implicit Euler time stepping scheme. Computational effort is reduced notably through techniques that enable spatial and temporal adaptivity, through a standard multigrid method as well as through a problem-oriented sparse-matrix storage concept. This study provides a suitable basis for the modeling and simulation of three-dimensional field scale problems as well as enhanced SVE techniques that use e.g. thermal energy or oxidative chemicals.

1 INTRODUCTION
Soil vapor extraction (SVE), also known as soil venting, is the standard in-situ clean-up technique targeting the removal of volatile organic compounds (VOCs) from the unsaturated zone: An induced gas flow towards vertical or horizontal drilled wells causes the evaporation of the nonaqueous phase liquid (NAPL), the volatilization of the contaminants dissolved in soil water and the desorption of the contaminants from the solid particles.

Accompanied with field and laboratory experiments, numerical simulations can lead to a better understanding of the physical and chemical aspects that describe an SVE system and can improve the identification of dominant parameters and processes that control the effectiveness of the remediation. This will support necessary technical enhancements and optimization.

The objective of this study is the development of a numerical model for the investigation of field- and laboratory-scale vapor extraction operations. Several authors have worked on the SVE technique both numerically and experimentally (Rathfelder et al. 1991; Armstrong et al. 1994; Fischer et al. 1996; Gerke et al. 1999; Ng & Mei 1999; Pennington et al. 1999). The model described here solves two- and three-dimensional flow and transport equations of a non-isothermal multicomponent/multiphase SVE system. After the theoretical analysis describing the mathematical modeling and numerical solution scheme, the model is applied to a two-dimensional laboratory test problem.

2 MATHEMATICAL MODELING
We are concerned here with the non-isothermal multicomponent gas flow in the unsaturated zone, the energy and mass transfer of the components between the gas phase ($g$), the water phase ($w$) and the solid phase ($s$). Pure phase of NAPL is absent. Such cases are considered to be critical, because they are characterized by low removal rates of VOCs and consequently by long cleanup times (Armstrong et al. 1994; Kalieris & Croisé 1997; Fischer et al. 1998). We neglect infiltration events and assume the water phase to be immobile in time. The soil matrix is incompressible.

2.1 Balance Equations
If volume averaged balance equations for the system are considered, then the mass balance equation for component $\kappa$ is

$$\frac{\partial}{\partial t} \left( S_g \rho_g X_g^\kappa \right) + \nabla \cdot \left[ \phi S_g \left( \rho_g v_g X_g^\kappa - F_g^\kappa \right) \right] = r_g^\kappa + m_g^{\kappa \beta}, \quad (1)$$
the total mass balance equation is
\[
\frac{\partial}{\partial t} (S_g \rho_g) + \nabla \cdot (\phi S_g \rho_g \mathbf{v}_g) = r_g + m_{g\beta},
\]
and the energy balance equation is
\[
\frac{\partial}{\partial t} (S_g \rho_g h_g) + \nabla \cdot \left[ \phi S_g \left( \rho_g \mathbf{v}_g h_g - F^h_g \right) \right] = s_g + q_{g\beta},
\]
where \( \rho_g \) is the density of the gas phase and is given by the ideal gas law. The following additional constraints have to be fulfilled:
\[
\begin{align*}
S_g + S_w &= 1, \\
\sum_{\alpha \in \{g,w,s\}} m_{g\beta} &= 0, \\
\sum_{\alpha \in \{g,w\}} m_{\alpha\beta} &= 0, \\
\sum_{\alpha \in \{g,w\}} q_{\alpha\beta} &= 0,
\end{align*}
\]
where \( \phi \) is the porosity, \( S_g \) and \( S_w \) are the gas and water saturations, \( X_j^k \) is the mass fraction of component \( k \) in the gas phase, \( \mathbf{v}_g \) is the velocity vector of the gas phase, \( F^h_g \) is the dispersive mass flux, \( r_g^h \) is the volumetric mass generation of component \( k \), \( m_{g\beta} \) is the volumetric rate of mass transfer between the gas phase and phase \( \beta \) of component \( k \), \( h_g \) is the specific enthalpy of the gas phase, \( m_{g\beta} \) is the volumetric rate of heat transfer between the gas phase and phase \( \beta \).

### 2.2 Advective Flux

The intrinsic velocity vector of the gas phase is estimated by Darcy’s Law (volume averaged momentum equation) assuming the gravity potential to be negligible:
\[
\phi S_g \mathbf{v}_g = \frac{k_{rg}}{\mu_g} \nabla \rho_g,
\]
where \( k_{rg} \) is the relative permeability, \( \mathbf{K} \) is the intrinsic permeability tensor, \( \mu_g \) is the gas phase pressure, \( \phi S_g \) is the volumetric rate of mass transfer between the gas phase and phase \( \beta \) of component \( k \), and \( h_g \) is the specific enthalpy of the gas phase.

### 2.3 Dispersive Mass and Energy Flux

The dispersive mass and energy fluxes for the gas phase are written as
\[
\phi S_g \mathbf{F}^m_g = \left( \mathbf{D}_g + D^k_g \right) \left( \rho_g \nabla X_g^k \right)
\]
and
\[
\phi S_g \mathbf{F}^h_g = D_g \left( \rho_g \nabla h_g \right).
\]

### 2.4 Interfacial Mass and Energy Transfer

Interfacial mass transfer is described by the two-flux theory (Bird et al. 1960; Welty et al. 1984; McCabe et al. 1993; Schlünder 1996), which assumes that mass transfer between phases is related to the diffusive fluxes through their interfacial viscous films. Setting the volumetric rate of mass transfer to the interface equal to the volumetric rate of mass transfer from the interface, it follows according to the linearized form of Fick’s first law that
\[
m_{\alpha\beta}^k = \frac{a_{\alpha\beta}}{l_{\alpha}} \left( \rho_{\alpha} X_{\alpha}^k - (\rho_{\alpha} X_{\alpha}^k)_{ph} \right)
\]
and

\[ m_{\alpha\beta}^K = \frac{a_{\alpha\beta} D_{\beta}^8}{l_{\beta}} \left( (\rho_\beta X_{\alpha}^K)_{ph} - \rho_\beta X_{\beta}^K \right), \quad (13) \]

where \(a_{\alpha\beta}\) is the volumetric interfacial area, evaluated by Rose & Bruce (1949), \(l_{\alpha}\) and \(l_{\beta}\) are the viscous film widths, \((\rho_\alpha X_{\alpha}^K)_{ph}\) and \((\rho_\beta X_{\beta}^K)_{ph}\) are the concentrations at the interfacial contact area.

The volumetric mass transfer rate can also be set equal to an overall mass transfer rate coefficient \(\gamma_{\alpha\beta}^K\) times an overall driving force:

\[ m_{\alpha\beta}^K = \gamma_{\alpha\beta}^K (\rho_\alpha X_{\alpha}^K - (\rho_\alpha X_{\alpha}^K)_{eq}), \quad (14) \]

where \((\rho_\alpha X_{\alpha}^K)_{eq}\) is the fictitious \(\alpha\) phase concentration in thermodynamic equilibrium with phase \(\beta\). Equation (14) is related to equation (12) and (13) by

\[ \frac{1}{\gamma_{\alpha\beta}^K} = \frac{l_{\alpha}}{a_{\alpha\beta} D_{\alpha}^8} + \frac{l_{\beta}}{a_{\alpha\beta} D_{\beta}^8} \left( \frac{(\rho_\alpha X_{\alpha}^K)_{ph} - (\rho_\alpha X_{\alpha}^K)_{eq}}{(\rho_\beta X_{\beta}^K)_{ph} - (\rho_\beta X_{\beta}^K)_{eq}} \right). \quad (15) \]

If thermodynamic equilibrium is assumed at the contact area between the viscous films, it follows:

\[ \frac{1}{\gamma_{\alpha\beta}^K} = \frac{1}{a_{\alpha\beta} \gamma_{\alpha}^K} + \frac{1}{a_{\alpha\beta} \gamma_{\beta}^K} \left( \frac{(\rho_\alpha X_{\alpha}^K)_{ph} - (\rho_\alpha X_{\alpha}^K)_{eq}}{(\rho_\beta X_{\beta}^K)_{ph} - (\rho_\beta X_{\beta}^K)_{eq}} \right). \quad (16) \]

where \(\gamma_{\alpha}^K\) and \(\gamma_{\beta}^K\) are the \(\alpha\)- and \(\beta\)-side mass transfer coefficients.

These, more exactly the viscous film widths, are dependent on the flow velocity of the phases and their film viscosities. Hence, for operational applications of the SVE technique, reliable data for the mass transfer coefficients might not be available. To resolve this problem, dimensional analysis can be used to formulate a set of dimensionless variables that are related to appropriate system variables and that facilitate a description of the process.

To do so, the \(\alpha\)- and \(\beta\)-side mass transfer coefficients are correlated in their dimensionless form, the so-called Sherwood number

\[ Sh_{\alpha} = \frac{\gamma_{\alpha}^K d_p}{D_{\alpha}^8}, \quad Sh_{\beta} = \frac{\gamma_{\beta}^K d_p}{D_{\beta}^8}, \quad (17) \]

to the respective Reynolds number

\[ Re_{\alpha} = \frac{\rho_\alpha u d_p}{\mu_{\alpha}}, \quad Re_{\beta} = \frac{\rho_\beta u d_p}{\mu_{\beta}}, \quad (18) \]

and Schmidt number

\[ Sc_{\alpha} = \frac{\mu_{\alpha}}{\rho_\alpha D_{\alpha}^8}, \quad Sc_{\beta} = \frac{\mu_{\beta}}{\rho_\beta D_{\beta}^8}, \quad (19) \]

i.e. \(Sh_{\alpha} = Sh(Re_{\alpha},Sc_{\alpha})\) and \(Sh_{\beta} = Sh(Re_{\beta},Sc_{\beta})\), where \(d_p\) is the mean grain size.

These dimensionless expressions have been widely used to aid in the description of mass and energy transfer phenomena (Friedlander 1957; Bird et al. 1960; Bowman et al. 1961; Miller et al. 1990; Sztakowski et al. 1994; Wilkins et al. 1995; Schlünder 1996).

![Figure 1](image-url)

Figure 1: Experimental setup of Fischer et al. (1996)

The two-film theory together with dimensional analysis is used analogously for the modeling of the interfacial energy transfer.

To estimate the fictitious gas phase concentration at thermodynamic equilibrium \((\rho_g X_g^voc)_{eq}\) for VOC gas-water phase mass transfer, we use the following relationship, derived from Henry’s Law, ideal gas law and Dalton’s Law:

\[ H_{vw}^voc := \frac{(\rho_g X_g^voc)_{eq}}{\rho_w X_w^voc} = \frac{h_{vw}^voc}{M_w RT \sum_{i=1}^{n} \frac{X_i}{M_i}}, \quad (20) \]

where \(R\) is the ideal gas constant, \(h_{vw}^voc\) is the Henry coefficient, which in turn results from an integration of the Clausius-Clapeyron differential equation (Heron et al. 1998).

For \(H_2O\) gas-water phase mass transfer, the following derivation, obtained from Raoult’s Law, the ideal gas law and Dalton’s Law, is used:

\[ R_{vw}^{H_2O} := \frac{(\rho_g X_g^{H_2O})_{eq}}{\rho_w X_w^{H_2O}} = \frac{p^{H_2O}}{\rho_w RT \sum_{i=1}^{n} \frac{X_i}{M_i}}, \quad (21) \]

where \(p^{H_2O}\) is the saturation vapor pressure, which in turn results from an integration of the Clausius-Clapeyron differential equation (Helmig 1997; Moore & Hummel 1983).

For VOC water-solid mass transfer, the distribution coefficient \(K_{D}^{voc}\), a linear Freundlich isotherm, can be used:

\[ K_{D}^{voc} := \frac{X_s^{voc}}{(\rho_w X_w^{voc})_{eq}}. \quad (22) \]
3 NUMERICAL SOLUTION

There are several possibilities for discretizing the system (1),(2),(3). The method of lines approach (MOL) discretizes in space and treats the resulting discrete system of ordinary differential equations by classical ODE procedures. Alternatively, one can discretize first in time and then in space. This is known as Rothe’s method, see (Bornemann 1992; Wagner 1998; Lang 1999) and the references there. A further possibility is the simultaneous discretization in space and time, see e.g. Eriksson & Johnson (1995).

For our computational results, we have used the software framework UG (Bastian et al. 1997), which allows for the parallel adaptive solution of a large variety of partial differential equations in two and three space dimensions. For convection-diffusion-reaction systems, it provides both the MOL approach and the Rothe method in an adaptive setting. For the results from section 4, the MOL approach is used. The spatial discretization is done by a finite volume method (see section 3.1) which is applied inside an implicit Euler scheme (see section 3.2).

3.1 Spatial discretization

For discretization in space, we use a vertex-centered finite volume scheme, also called box method, which we want to sketch briefly. We assume that we are given a grid \( \mathcal{T} \) consisting of vertices \( v_\lambda, \lambda \in \Lambda \) which are corners of elements (triangles and/or quadrangles) \( e_\nu, \nu \in \mathcal{V} \). Here \( \Lambda \) and \( \mathcal{V} \) are suitable index sets. By connecting the midpoints of element sides with the centers of elements, one obtains a dual grid consisting of boxes \( B_\lambda \) around the vertices \( v_\lambda \). Then, a discrete system is obtained by integrating (1),(2),(3) over the boxes \( B_\lambda \) and replacing the unknowns \( p_\nu \), \( X_\nu \), and \( h_\nu \) by approximations that are piecewise linear/bilinear on triangle/quadrangle elements. This approach is well-known and can be found at many places (see e.g. Bastian (1999) for a detailed description). The diffusion tensors and convection vector fields in (1) and (3) are assumed to be constant on elements and are evaluated by midpoint rules. For the convective terms, full upwinding is used to avoid spurious oscillations.

Figure 2: Upper and lower bounds of the Peclet number \([-\] \) at the grid scale versus tank elevation \([m]\)

Figure 3: Comparison with experimental results for TCE and 1.1.1.-TCA at the sampling ports 13 (\( S_w = 0.38 \)) and 23 (\( S_w = 0.17 \)).
3.2 Time stepping scheme

Let \( Y(t_k) = (p_g(t_k), X_g^\alpha(t_k), h_g(t_k)) \) be an approximation to the solution of equations (1),(2),(3) discretized in space with the finite volume scheme from the previous section. We then use the following time-stepping scheme to obtain a discrete approximation \( Y(t_{k+1}) = (p_g(t_{k+1}), X_g^\alpha(t_{k+1}), h_g(t_{k+1})) \) at time \( t_{k+1} = t_k + \Delta t \).

(i) We replace the time derivative in the space-discretized form of (1) and (3) with a backward difference (implicit Euler method). The diffusion coefficients are chosen to depend on \( \beta(t_k) \) and the flow field is obtained by (5) applied to \( p_g(t_k) \). Due to the chemical reaction, the discrete equations will still be nonlinear in general. Applying Newton’s method, we end up with linear systems which we solve by a multigrid iteration with a block Gauss-Seidel smoother, where the blocks correspond to all values \( \beta(t_k) \) at one vertex \( \nu_\lambda \).

(ii) [Time step control] Starting again from the old solution \( Y(t_k) \) we perform two time steps with size \( \Delta t/2 \) to obtain a more accurate solution \( Y'(t_{k+1}) = (p'_g(t_{k+1}), X'_g^\alpha(t_{k+1}), h'_g(t_{k+1})) \). The time step is halved, if \( \|Y(t_{k+1}) - Y'(t_{k+1})\|_2 \) is larger than \( TOL \Delta t \) (or if the Newton or the multigrid iteration converge too slowly). On the other hand, if \( \|Y(t_{k+1}) - Y'(t_{k+1})\|_2 \) is below \( TOL' \Delta t \) with some \( TOL' < \frac{TOL}{2} \), the size of the following time step is doubled. Here, \( TOL \) and \( TOL' \) are given tolerances for the local error.

(iii) We neglect the time-derivative in (2). This is reasonable, because density changes are slow outside of a short transitional phase. Then, we linearize the equation by using \( X_g^\alpha(t_k), h_g(t_k) \) in the permeability coefficient. The resulting scalar elliptic equation is solved again with a multigrid iteration.

(iv) [Grid adaption] We use an hierarchical error estimator measuring the square of the differences between the values of \( X_g^\alpha(t_{k+1}), h_g(t_{k+1}) \) and \( \nu_\lambda(t_{k+1}) \) on subsequent levels. This local quantity measures the interpolation error and can be used as an indicator for refinement and coarsening. An upper limit for the number of grid levels avoids excessive refinement along sharp fronts.

Let us end this description with some remarks: First, the linear systems which have to be solved in step (i) have a very special structure which can be used to improve storage requirements and computational speed, see Neuss (1999). Second, for more difficult problems, it is usually not trivial to obtain optimal multigrid convergence. Problems may occur, for example, if we have large variations in the permeability coefficients. Here, modified multigrid schemes based on algebraic information have to be used. We do not want to go into detail, because we will not encounter this kind of problem for the results presented in the next section.

4 RESULTS AND DISCUSSION

The numerical simulation model was verified using the SVE experiments of Fischer et al. (1996), which were carried out at different water contents in a tank (Figure 1) using a homogeneous packing of quartz. Figure 4: Comparison with experimental results for TCE and 1.1.1.-TCA at the sampling ports 33 \( (S_w = 0.11) \) and 43 \( (S_w = 0.08) \).
sand as the model soil. In this experiment four chlorinated VOCs were used as the model components. Liquid phase was absent. Gas phase concentrations were measured at several locations with different water saturations during each experiment. The components did not adsorb onto the sand. Volatilization was the key process for VOC removal. More details about the experimental procedures applied in the tank venting experiments are given by Fischer et al. (1996) and Fischer et al. (1998).

The phase-specific space and time dependent Sherwood and Nusselt numbers, the mass and energy transfer coefficients respectively, were estimated according to a correlation of Bowman et al. (1961), which was analytically derived for transfers from fluid and solid spheres at low Reynolds numbers:

\[ Sh = 2 + \frac{9}{16} Re Sc + \frac{9}{64} Re^2 Sc^2 + \ldots \]  

(23)

The longitudinal and transversal dispersivities were related to the size of the elements occurring on the finest grid level \( \alpha_{LT} = \alpha_T = 1.125 \cdot 10^{-2} \text{ m} \). All further modeling parameters were based on the given experimental measurements or obtained from literature cited data (Lide 1995).

Gas phase transport at the grid scale was dominated by hydrodynamic dispersion. The spatial variation of the Pelet number, calculated from equation (5), (10) and (11), was related to the decreasing water saturation \( S_w \) along the elevation axis (Figure 2). Simultaneously, interfacial mass transfer rate coefficients decreased with decreasing water saturation \( S_w \). Hence, at elevations with a very high water saturation (e.g. sampling port 13) vapor pressures were of greater influence on the interfacial mass transfer than at elevations with a very low water saturation (e.g. sampling port 43). Such spatial distributed and component-specific effects can be used, e.g., for the determination of critical gas phase velocities and length scales, i.e. for the estimation of optimal SVE pumping rates.

A drawback of our detailed approach is the large number of parameters that are required to describe the system. Nevertheless, we generally succeeded in matching the measured TCE and 1.1.1.-TCA concentrations at the different sampling ports for the experiment V2 (Figure 3 and 4) without applying any curve fitting. Furthermore the detailed model allows for the implementation of enhanced remediation techniques that use e.g. thermal energy or oxidative chemicals.

5 CONCLUSIONS
We described a non-isothermal multicomponent/multiphase model which can represent spatially distributed effects that are related to coupled physical and chemical processes. This kind of information can be used to improve the performance of a soil vapor extraction system.

Our numerical scheme is adaptive in time and space and uses an optimal solver (multigrid). It is embedded inside a flexible framework, which allows to treat a wide range of reactive flow problems. Parallelism is supported, even if we did not use it yet for simulating soil vapor extraction systems. In the future, we will apply this technique to real-world situations where parallel computations may be necessary.

6 NOTATION

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
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<tbody>
<tr>
<td>( a_{\alpha\beta} )</td>
<td>vol. surface area between phase ( \alpha ) and ( \beta ), ( \frac{1}{m} ).</td>
</tr>
<tr>
<td>( \alpha_L )</td>
<td>longitudinal dispersivity, ( m ).</td>
</tr>
<tr>
<td>( \alpha_T )</td>
<td>transversal dispersivity, ( m ).</td>
</tr>
<tr>
<td>( F_c^g )</td>
<td>gas phase dispersive mass flux, ( \frac{k_g}{s} ).</td>
</tr>
<tr>
<td>( F_h^g )</td>
<td>gas phase dispersive heat flux, ( \frac{W}{m^2} ).</td>
</tr>
<tr>
<td>( D_g )</td>
<td>dispersion tensor, ( \frac{m^2}{s} ).</td>
</tr>
<tr>
<td>( d_p )</td>
<td>mean grain size, ( m ).</td>
</tr>
<tr>
<td>( \gamma_\alpha^g )</td>
<td>multicomponent diffusivity, ( \frac{m^3}{s} ).</td>
</tr>
<tr>
<td>( \gamma_\alpha^{\alpha\beta} )</td>
<td>( \alpha )-side mass transfer coefficient, ( \frac{m}{s} ).</td>
</tr>
<tr>
<td>( h_\alpha )</td>
<td>( \alpha )-side specific enthalpy, ( \frac{J}{kg} ).</td>
</tr>
<tr>
<td>( h^{voc} )</td>
<td>Henry coefficient, ( \frac{P_a}{m^3/mol} ).</td>
</tr>
<tr>
<td>( k_r^g )</td>
<td>gas phase relative permeability.</td>
</tr>
<tr>
<td>( K )</td>
<td>intrinsic permeability tensor, ( m^2 ).</td>
</tr>
<tr>
<td>( K^{voc}_D )</td>
<td>distribution coefficient, ( \frac{m^3}{kg} ).</td>
</tr>
<tr>
<td>( l_\alpha )</td>
<td>( \alpha )-side viscous film width, ( m ).</td>
</tr>
<tr>
<td>( m )</td>
<td>van Genuchten parameter.</td>
</tr>
<tr>
<td>( m_{\alpha\beta} )</td>
<td>total interfacial vol. rate of mass transfer, ( \frac{k_g}{m^2/s} ).</td>
</tr>
<tr>
<td>( m_{\alpha\beta}^{\alpha\beta} )</td>
<td>comp. ( \alpha )-side interfacial vol. rate of mass transfer, ( \frac{k_g}{m^2/s} ).</td>
</tr>
<tr>
<td>( \mu_g )</td>
<td>multicomponent gas viscosity, ( Pa \cdot s ).</td>
</tr>
<tr>
<td>( p_g )</td>
<td>gas phase pressure, ( Pa ).</td>
</tr>
<tr>
<td>( p_{H_2O} )</td>
<td>( H_2O ) saturation vapor pressure, ( Pa ).</td>
</tr>
<tr>
<td>( \phi )</td>
<td>porosity.</td>
</tr>
<tr>
<td>( q_{\alpha\beta} )</td>
<td>interfacial vol. rate of heat transfer, ( \frac{W}{m^2} ).</td>
</tr>
<tr>
<td>( r_{\alpha\beta} )</td>
<td>vol. total mass generation, ( \frac{k_g}{m^2/s} ).</td>
</tr>
<tr>
<td>( r_\alpha^{\alpha\beta} )</td>
<td>comp. ( \alpha )-side vol. mass generation, ( \frac{k_g}{m^2/s} ).</td>
</tr>
<tr>
<td>( R )</td>
<td>ideal gas constant, ( \frac{Pa m^3}{mol} ).</td>
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<tr>
<td>( Re_\alpha )</td>
<td>( \alpha )-side Reynolds number.</td>
</tr>
<tr>
<td>( \rho )</td>
<td>density of phase ( \alpha ), ( \frac{kg}{m^3} ).</td>
</tr>
<tr>
<td>( s_\alpha )</td>
<td>( \alpha )-side phase vol. heat generation, ( \frac{W}{m} ).</td>
</tr>
<tr>
<td>( S_a )</td>
<td>saturation of phase ( \alpha ).</td>
</tr>
<tr>
<td>( S_{ae} )</td>
<td>emergence/extinction point.</td>
</tr>
<tr>
<td>( S_w )</td>
<td>residual water saturation.</td>
</tr>
<tr>
<td>( S_{\alpha\beta} )</td>
<td>( \alpha )-side Schmidt number.</td>
</tr>
<tr>
<td>( Sh_\alpha )</td>
<td>( \alpha )-side Sherwood number.</td>
</tr>
<tr>
<td>( T_\alpha )</td>
<td>( \alpha )-phase temperature, ( K ).</td>
</tr>
<tr>
<td>( \phi_g )</td>
<td>gas phase velocity vector, ( m ).</td>
</tr>
<tr>
<td>( X_\alpha )</td>
<td>mass fraction of comp. ( \kappa ) in phase ( \alpha ).</td>
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