

THE UNIVERSITY OF CALGARY

Dispersion Models in Reservoir Simulation

by

Bruce F. Kohse

A DISSERTATION

SUBMITTED TO THE FACULTY OF GRADUATE STUDIES

IN PARTIAL FULFILLMENT OF THE REQUIREMENTS FOR THE

DEGREE OF

DOCTOR OF PHILOSOPHY

DEPARTMENT OF

CHEMICAL AND PETROLEUM ENGINEERING

CALGARY, ALBERTA

APRIL, 1994

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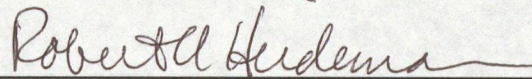
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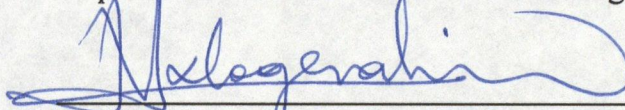


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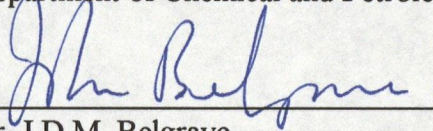
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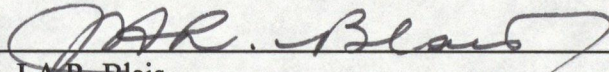
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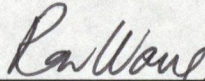
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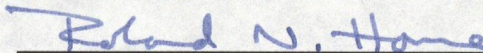
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ABSTRACT

Field experience and laboratory investigations have shown that dispersion is an important factor in miscible displacement oil recovery processes. Dispersion in these processes can be due to a number of mechanisms, including: molecular diffusion, microscopic convective dispersion and macroscopic dispersion. Recent experimental work performed at the Shell Canada Calgary Research Center has shown that high levels of dispersion can result from turbulent mixing effects occurring when the miscible solvent and reservoir oil exhibit a large volume change on mixing. Mixing via any one or combination of these mechanisms can be characterized by an effective dispersion coefficient.

This dissertation describes methods for modeling displacements with dispersion using a compositional simulator. A standard simulator, which does not treat dispersion explicitly, is used as the base to which dispersion models are added. The dispersion models are derived from Fick's first law and second law (i.e., the diffusion equation) employing effective dispersion coefficients in place of the usual diffusion coefficient. The solutions of the diffusion equation required for these models are derived here using the Green's function method.

The first law and second law models both prove capable of predicting dispersion in three example systems tested. The total level of dispersion predicted by the simulator is dependent on the level of numerical dispersion and the physical dispersion model chosen. Techniques for numerical dispersion control also limit the prediction of physical dispersion. A front tracking model based on the standard error function solution of the diffusion equation is developed, and is found to significantly alleviate the numerical dispersion problems for one dimensional simulations.

ACKNOWLEDGEMENTS

- The first acknowledgement must be made to my wife, Lori, for her patience and support throughout the course of this work.
- Thanks are due to the staff of the recovery processes research group at the Shell Canada Calgary Research Center: Nancy Lever, Cor van Kruijsdijk, Laurie Sibbald and Doug Malcolm, for initiating the project and allowing me access to the research facility. Special thanks to Laurie for providing the experimental data for analysis, and Cor for introducing me to the analytical modeling methods used in this work.
- I would like to acknowledge Shell Canada for financial support and access to computing facilities.
- Many thanks of course to my supervisor, Dr. Robert Heidemann, for guidance, assistance and motivation throughout all of my graduate work.

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NOMENCLATURE

α, b	equation of state constants
c_1, c_2	equation of state constants
d_p	average particle size (m)
D_m	effective multicomponent diffusion coefficient of component m (m ² /s)
f	fugacity (Pa)
F	formation electrical resistivity factor
g	gravitational acceleration (m/s ²)
G	time domain source function
$\overline{G}$	Laplace domain source function
I_w	well index (m ³ /Pa·s)
$\mathbf{j}$	mass diffusive flux vector field (kg/m ² s)
$J_{i,k}$	element of Jacobian matrix
K	permeability (m ²)
K_l	total longitudinal dispersion coefficient (m ² /s)
K_t	total transversedisersion coefficient (m ² /s)
k_{rj}	relative permeability of phase j
L	mole fraction liquid in the hydrocarbon system
l_i	length of grid block i (m)
$\mathbf{m}$	mass flux vector field (kg/m ² s)
n_b	number of grid blocks
n_c	number of components
n_m	mole number of component m
P	pressure (Pa)
P_c	critical pressure (Pa)
q	molar source rate (kmol/s)
$\hat{q}$	molar source rate per unit volume (kmol/m ³ s)
$\tilde{q}$	mass source rate per unit volume (kg/m ³ s)
Q	volumetric flow rate (m ³ /s)

R	universal gas constant (Pa·m ³ /kmol·K)
S	phase saturation (volume fraction)
T	temperature (K)
T_c	critical temperature (K)
T_x	transmissibility in the x direction (kmol/Pa·s)
t	time (s)
u	velocity (m/s)
$\mathbf{u}$	velocity vector field (m/s)
V	mole fraction vapor in the hydrocarbon system
V_b	grid block volume (m ³)
v	specific molar volume (m ³ /kmol)
v_c	critical molar volume (m ³ /kmol)
x, y	coordinate directions
x_m	mass fraction of component m
y_{mj}	mole fraction of component m in phase j
Z	compressibility factor
z	vertical thickness (m)
z_m	global mole fraction of component m
ρ	molar density (kmol/m ³)
ρ_m	molar density of component m (kmol/m ³)
$\tilde{\rho}$	mass density (kg/m ³)
μ	viscosity (Pa·s)
σ	inhomogeneity factor
ϕ	porosity
λ_j	mobility of phase j , Kk_{rj}/μ (1/Pa·s)
ω_m	acentric factor for component m

SUBSCRIPTS

o	oil
g	gas
w	water

s solvent

SUPERSCRIPTS

l iteration level

n time step level

1. INTRODUCTION

The process of displacing oil from reservoirs with a miscible gaseous injectant has been examined from many perspectives. Laboratory investigations, field experience and mathematical modeling have all contributed to the current state of understanding of this process. In this chapter, a review of the physics of miscible displacement is presented, including a description of recent experiments which suggest that an "enhanced dispersion" effect which has not been studied before may play an important role in the mixing of solvent and oil in the reservoir. A review of modeling techniques used for miscible flood simulation, and a proposal for the development and implementation of new dispersion models in existing compositional reservoir simulators is given.

1.1. REVIEW OF MISCIBLE DISPLACEMENT PHYSICS

1.1.1. PHASE BEHAVIOR

The equilibrium phase behavior of mixtures of reservoir oil and gaseous solvent is of primary importance in the design of miscible displacement processes. The fundamentals of miscible processes are described in Stalkup (1983). For a first contact miscible process, the solvent mixes with the reservoir oil completely in all proportions and a single phase mixture results regardless of the relative amounts of the fluids. For a given oil/solvent pair, the minimum pressure at which all mixtures lie outside the two-phase region is referred to as the first contact miscibility pressure; a decrease in pressure below this point would result in some mixtures of oil and solvent splitting into two phases.

It is possible to obtain miscibility at pressures lower than the first contact miscibility pressure via dynamic or multiple contact miscibility. One mechanism for achieving this is the vaporizing gas drive, in which miscibility is obtained at the front of the

solvent bank displacing the oil. A lean solvent which is not miscible with the oil on first contact is injected, resulting in the formation of two phases. The vapor phase is enriched with intermediate components from the oil, and as this vapor phase moves forward and contacts more fresh oil, the continuous enrichment allows the vapor to achieve the critical composition and become miscible with the reservoir oil.

The other mechanism for achieving multiple contact miscibility is the condensing gas drive process, in which miscibility is obtained at the tail of a transition zone between the original reservoir oil and the injected solvent. A rich gas is injected, forming two phases and transferring some intermediates from the injectant to the oil. The equilibrium gas moves forward, leaving the enriched oil to be further contacted with fresh solvent until the oil is enriched to the point where it becomes miscible with the injection gas. For a typical injection gas which does not contain the middle heavy fractions present in the oil, the gas will enrich the oil in the light intermediate range while stripping the heavier fractions. This results in miscibility being achieved within the transition zone where the gas front behaves like a vaporizing gas drive and the tail as a condensing gas drive (Zick, 1986).

For the condensing gas drive, the solvent must contain intermediate molecular weight hydrocarbons, typically ethane through butane, to enrich the reservoir oil. The lean gas used for the vaporizing gas drive may be natural gas, flue gas or nitrogen. CO_2 is also used as a solvent which attains miscibility through a vaporizing type process, however, it extracts much higher molecular weight hydrocarbons than lean gas solvents (Stalkup, 1983; p. 14). The use of CO_2 as a solvent also raises the possibility that two liquid, or two liquid plus vapor equilibria will be attained. The effect of multiple phase equilibria on the displacement process must be taken into account (Gardner et al., 1981). The appearance of an equilibrium solid phase, asphaltenes, has been observed for intermediate molecular

weight hydrocarbon and CO₂ solvents (Bossler and Crawford, 1959; Shelton and Yarborough, 1977). Severe asphaltene precipitation may reduce permeability in the reservoir, or even cause plugging in producing wells.

Accurate models of the equilibrium phase behavior of the reservoir oil and proposed solvent are required to determine if miscibility will be attained, and if so, through what mechanism. The extent of multiple phase equilibrium behavior and solids precipitation for a given oil/solvent pair must also be known for the design of a miscible process. The degree of mixing of oil and solvent and the rate of mass transfer between the phases will have an impact on process design elements such as the volume of the miscible slug to be injected and injection rates. The mechanisms of mixing are discussed in the following section.

1.1.2. DISPLACEMENT BEHAVIOR

1.1.2.1. Mobility Ratio

One of the most important factors in displacing an oil from a reservoir with a miscible gaseous solvent is the mobility ratio of the displacement. Mobility is defined as the effective permeability of the rock to a fluid phase j which is given by the total permeability multiplied by the relative permeability for that phase, divided by the viscosity of that fluid (Stalkup, 1983; p. 31):

$$\lambda_j = \frac{Kk_{rj}}{\mu_j} \quad (1.1)$$

The mobility ratio, M , for any displacement process is defined as the mobility of the displacing fluid divided by that of the displaced fluid. For miscible processes, the gaseous solvent viscosity is always low in relation to the reservoir oil viscosity and the mobility ratio is always greater than one. Mobility ratios greater than unity are termed unfavorable

as the displacement front between the two fluids may be unstable, resulting in the growth of viscous fingers which greatly reduce the efficiency of the oil recovery process (Habermann, 1960). Viscous fingering is discussed in more detail later in this chapter.

In many situations, determination of the mobility ratio is quite complex. When there is no mobile water, the permeability of the rock to the oil and miscible solvent will be equal, thus the mobility ratio will reduce to the viscosity ratio of oil to solvent. In practical situations, however, mixing of solvent and oil will reduce the viscosity ratio, and the presence of mobile water will alter the relative permeability characteristics, necessitating the definition of an effective mobility ratio. When there is more than one displacing front, the motion of any front is affected by the mobility ration across that front and also by the mobilities and relative sizes of the other fluid regions in the reservoir.(Stalkup, 1983; p. 32).

1.1.2.2. Dispersion

Diffusion and dispersion of miscible fluids in porous media have been studied extensively since miscible flooding was first investigated as a means of enhanced oil recovery. Dispersion can have a detrimental effect on miscible displacements by dissipating the solvent slug sufficiently that miscibility is lost. On the other hand, dispersion can tend to mitigate the adverse effects of viscous fingering. The review by Perkins and Johnston (1963) investigates two factors affecting dispersion in porous media: molecular diffusion, and microscopic longitudinal and transverse dispersion due to flow through the medium. Macroscopic dispersion due to permeability heterogeneities on a scale larger than the individual pore size yet smaller than the gross reservoir features can also have a large impact on the fluid mixing (Stalkup, 1983; p. 32). These effects form the usual context for study and modeling of dispersion.

Greenkorn (1983; p. 190) presents a more detailed list of dispersion mechanisms in porous media:

1. Molecular diffusion: normally associated with time scales longer than those required for dispersion due to other mechanisms.
2. Mixing due to obstructions: tortuous flow channels in the porous medium cause fluid elements traveling at the same velocity to diverge in space.
3. Presence of auto-correlation in flow paths: incomplete connectivity of the medium causes dispersion, as not all pores are accessible to a fluid once it has entered a particular flow path.
4. Recirculation caused by local regions of reduced pressure: flow restrictions can create localized low pressure regions, resulting in a pressure gradient driving a fluid back into a region that it has flowed through already.
5. Macroscopic or megascopic dispersion: caused by reservoir heterogeneities which alter the gross streamlines of the fluid.
6. Hydrodynamic dispersion: due to the velocity profile in the pores, in which the fluid tends to adhere to the wall of the pore.
7. Eddies: if flow in a channel becomes turbulent, eddy mixing will result.

A discussion of the three main mechanisms of mixing: molecular diffusion, microscopic convective dispersion and macroscopic convective dispersion is given below.

In many recovery processes, molecular diffusion is assumed to be negligible in comparison to other dispersive forces. In the case of lean gas injection into fractured reservoirs, however, diffusion can result from concentration differences between the lean gas in the fracture and the hydrocarbon phase in the matrix rock (Saidi, 1987). For very

low permeability and highly fractured reservoirs, molecular diffusion could become the predominant recovery mechanism (Morel et al., 1990).

Mixing between two miscible fluids brought together in the absence of any external driving forces, e.g. pressure or temperature gradients, is assumed to proceed by molecular diffusion alone (Perkins and Johnston, 1963). This diffusive flux for any component i in a multicomponent mixture can be described by Fick's first law of diffusion written with an effective diffusion coefficient:

$$\mathbf{j}_i = -\tilde{\rho}D_i\nabla x_i \quad (1.2)$$

This equation is valid only if there is no volume change on mixing of the two fluids. The value of the effective diffusion coefficient depends on the local concentration of components in the mixture and temperature and pressure of the system (Lo and Sigmund, 1971). Application of Fick's law for reservoir conditions also requires that the diffusion coefficient be modified to account for the effects of the porous medium. Recognition of the analogy between electrical conductivity and diffusion in porous media allows a relation between the diffusion coefficient in a porous medium, D , and that in an open channel, D_o , to be written as (Perkins and Johnston, 1963):

$$\frac{D}{D_o} = \frac{1}{F\phi} \quad (1.3)$$

where F is the formation electrical resistivity factor and ϕ is the fractional porosity. The above equations describe the mixing of fluids in porous media in the absence of flow.

Microscopic convective dispersion results from both hydrodynamic dispersion caused by the velocity profile within the pores and mechanical mixing caused by the tortuous flow path fluid elements must take through the medium (Greenkorn, 1983; p. 184). Hydrodynamic longitudinal dispersion in thin tubes has been examined as a simple analog for flow within the pores of a porous medium. For the case of one fluid in a tube

being displaced by another fluid injected at one end of the tube, the concentration of injected fluid in the effluent can be determined simply by integration of the flow equation, provided there is no diffusion, the viscosity of the displacing fluid is equal to that of the resident fluid and the flow is laminar. When diffusion is considered, the size of the mixing zone will decrease compared to that obtained with convective dispersion alone. Taylor (1953) studied this phenomenon under certain conditions of tube size and fluid velocity such that diffusion would damp out radial concentration variations and a symmetrical longitudinal mixed zone would be established. The size of the mixed zone will grow as if a constant longitudinal dispersion coefficient for the system existed, given by the following equation

$$K_l = D_o + \frac{u^2 a^2}{48 D_o} \quad (1.4)$$

where a is the radius of the capillary tube. Dispersion coefficients in sand packs have been correlated with a similar relation (Perkins and Johnston, 1963) as follows:

$$\frac{K_l}{D_o} = \frac{1}{F\phi} + 0.5 \frac{u\sigma d_p}{D_o}; \frac{u\sigma d_p}{D_o} < 50 \quad (1.5)$$

where σ is an inhomogeneity factor and d_p is the average particle size. This relation is only valid for fluids of equal density and viscosity. Estimates of longitudinal dispersion coefficients can be obtained with this equation, recognizing that fluid saturations, density ratio, viscosity ratio and particle size distributions will affect the magnitude of the coefficient.

Flow through porous media will also cause fluids to be mixed by convective dispersion transverse to the direction of flow. As for longitudinal dispersion, the magnitude of this transverse dispersion is proportional to the average interstitial velocity.

A relation for the transverse dispersion coefficient, similar to that for longitudinal dispersion and subject to the same restrictions, is given by Perkins and Johnston (1963) as

$$\frac{K_t}{D_o} = \frac{1}{F\phi} + 0.0157 \frac{u\sigma d_p}{D_o}; \frac{u\sigma d_p}{D_o} < 10^4 \quad (1.6)$$

In general, at field displacement rates both microscopic convective dispersion and molecular diffusion may contribute to the longitudinal mixing of liquids, while molecular diffusion plays a larger role in the longitudinal mixing of gases. For transverse mixing in field displacements, molecular diffusion is the dominant mechanism of dispersion for all fluids (Stalkup, 1983; p. 35).

Heterogeneities of the porous media can also cause dispersion of fluids in the reservoir. Macroscopic dispersion refers to mixing caused by heterogeneities of the media larger than core scale. This can include strata of differing permeabilities, or permeability and porosity variations within individual strata. Regions of higher permeability will allow fluids to pass more easily, thereby spreading an initially uniform fluid front. Regions of higher porosity or dead end pore volume create greater capacitance in the reservoir and thus will retard the advancement of fluids. Since the scale of these heterogeneities is larger than can be represented in laboratory scale displacements, the effect of this macroscopic dispersion generally cannot be determined in core-flooding experiments. Difficulty in reservoir modeling occurs when the scale of these heterogeneities is smaller than the gross features which may be described in a simulation model, but are larger than core size.

Warren and Skiba (1964) used a Monte Carlo simulation technique to show that dispersion in a reservoir would be increased due to permeability variations alone and that the scale of the heterogeneities and the distribution function of the permeabilities both affected the amount of dispersion. The results of these simulations show that dispersion

caused by permeability variations can be modeled using a convection-diffusion type equation with an effective dispersion coefficient. Thus fluid mixing, whether it is caused by molecular diffusion, microscopic convective dispersion, macroscopic dispersion, or a combination of mechanisms, may be characterized by an effective dispersion coefficient.

1.1.2.3. Flow Regimes and Viscous Fingering

As mentioned earlier, displacing oil with a less viscous solvent may result in an unstable displacement front characterized by viscous fingers. The geometry of the process and the ratio of viscous to gravity forces will determine the degree to which viscous fingering will occur. For example, when a less dense solvent displaces oil in down-dipping strata, gravity acts to keep the oil and solvent separated, provided a critical displacement rate is not exceeded. In experiments on unfavorable mobility ratio displacements in vertical cross sections, four flow regimes have been identified depending on the value of the ratio of viscous to gravity forces (Stalkup, 1983; p. 37). This ratio is defined by

$$R_{v/g} = \frac{u\mu_o L/K}{\Delta\rho gh} \quad (1.7)$$

where $\Delta\rho$ refers to the difference in density between the oil and solvent, L is the length of the cross section and h is the vertical height. The first two regimes, at low viscous to gravity force ratios, are characterized by a single gravity tongue of solvent overriding the oil. As the viscous to gravity force ratio increases, a transition region develops where a main gravity tongue still forms but smaller fingers of solvent penetrate into the oil. The final flow regime is characterized by multiple fingers of solvent throughout the cross section with no large tongue of solvent overriding the oil.

When gravity does not affect the displacement, processes with favorable mobility ratios will have stable displacement fronts in which mixing between the fluids will take

place via the dispersion mechanisms discussed above. With unfavorable mobility ratios, however, the solvent front will become unstable and fingers of solvent will penetrate into the oil. The initiation of fingers is attributed to the presence of permeability heterogeneities (Stalkup, 1983; p. 40). As evidenced by experiments with glass bead packs, even porous media which are macroscopically homogeneous have microscopically random pore structure. These small variations in the pores are sufficient to initiate fingers in unfavorable mobility ratio displacements. In stable displacements, these irregularities in the flow are damped out by dispersion; in unstable displacements the flow irregularities are magnified and the fingers grow at a high enough rate that dispersion will not eliminate them.

Once fingers are initiated, their primary growth is in length; the higher the value of the mobility ratio, the faster the fingers will grow. Fingers grow in width by spreading due to transverse dispersion and also by merging with other fingers. Longitudinal dispersion is generally not important in the growth of finger length, however the rate of transverse dispersion can have a large effect on the degree of fingering (Stalkup, 1983; p. 41). A very high rate of transverse dispersion can stabilize a displacement by reducing the number of fingers.

Viscous fingers result in earlier breakthrough of solvent at production wells and consequent poorer oil recovery compared to stable displacements. Viscous fingering can also be viewed as a form of fluid mixing; although the oil and solvent remain segregated, the degree of fingering will affect the overall fraction of solvent in a given volume of reservoir rock. Thus, fingering and dispersion mechanisms will both contribute to the mixing of fluids in the reservoir.

1.2. "ENHANCED DISPERSION": AN ADDITIONAL MIXING MECHANISM IN MISCIBLE DISPLACEMENTS

Experimental work performed at the Shell Canada Calgary Research Center has indicated that additional mixing mechanisms may be active in miscible displacements (Sibbald et al., 1991). The two types of experiments used to examine mixing effects in oil/solvent contacting and the results obtained are summarized below.

1.2.1. VISUAL EXPERIMENT

Sibbald and his co-workers (1991) designed an apparatus to visually observe the process of live reservoir oil and fully miscible solvent mixing in the absence of external pressure and temperature gradients.

The equipment consisted of a glass tube of rectangular cross-section, 1 x 5 mm, with a notch drilled in one side at the midpoint. The tube was placed in a water bath at reservoir temperature and pressure. Live oil was pumped in one end of the tube until it reached the midpoint, displacing water through the notch into the surrounding vessel. Solvent was then injected slowly into the opposite end of the tube until all of the water was displaced through the notch and the gas and oil surfaces came into contact. The results of this experiment showed the solvent/oil interface moving rapidly in the direction of the solvent-filled portion of the tube. The growth of the mixing zone indicated by this interface movement was quantified by evaluating effective dispersion coefficients for several solvents. For all solvents the interface position was found to be a linear function of the square root of time, indicating that the process could be described with an effective dispersion coefficient. The dispersion coefficients calculated from these experiments were found to be in the range of 0.1 to 1.0 cm²/s, several orders of magnitude larger than molecular diffusion coefficients.

A proposed explanation for this rapid dispersion (Sibbald et al., 1991) is that a convective mixing process was occurring on contact between the two phases. A possibly related effect involving the enhancement of diffusion by natural convection in supercritical fluids has been documented by Debenedetti and Reid (1986). A suggested driving force for a convective effect in the visual experiment is a negative volume change on mixing of the two phases. A decrease in volume on mixing at a constant pressure implies a local pressure decrease on mixing at a constant volume. This pressure decrease would create local pressure gradients driving fluids toward the mixed zone. As the solvent is more mobile than the oil, the solvent moved most readily into the mixed zone. The resulting single phase mixed fluid will grow into the region vacated by the solvent as was observed in the experiments.

1.2.2. TAYLOR DISPERSION EXPERIMENT

A high temperature and pressure Taylor dispersion apparatus was constructed by Sibbald et al. (1991) to further quantify the effect observed in the visual experiment. The equipment consisted of a length of capillary tubing with inside diameter of 0.8 mm located in a temperature controlled oil bath. A sample loop of capillary tubing containing live oil or other solute was also located in the oil bath. Solvent flowing through the capillary tube was diverted through the sample loop via a chromatograph switching valve, thus the slug of solute was carried through the tubing and dispersion with the solvent took place at both the leading and trailing edges of the slug. The solvent flow rate was 0.2 mL/hour and the length of capillary tubing downstream of the sample loop was 619 cm.

The experiment was performed first with a live oil sample slug and ethane solvent at reservoir conditions of 22.75 MPa and 98.9°C. At these conditions, the two fluids are completely miscible and have a significant negative volume change due to mixing. A

second run was performed using *n*-octane as the solute slug and *n*-hexane as solvent at a pressure of 1.1 MPa and an ambient temperature of 20°C. In this case, the two fluids are completely miscible but exhibit no appreciable volume change on mixing. Following the development of Taylor (1953) for calculating dispersion coefficients under ideal mixing and laminar flow conditions in an apparatus of this type, approximate values of the dispersion coefficients for these two runs were calculated. The coefficients obtained were 1.0×10^{-2} cm²/s for the live oil/ethane case, and 6.0×10^{-4} cm²/s for the *n*-octane/*n*-hexane case. These data indicate that an enhancement to dispersion of the type seen in the visual experiment was occurring in the live oil/ethane experiment which was not occurring with the *n*-octane/*n*-hexane pair. Although the dispersion coefficient for *n*-octane/*n*-hexane was larger than the usual upper limit of 10^{-4} cm²/s for liquid-liquid diffusion, it was at least on the same order of magnitude, while the coefficient for live oil and ethane was obviously much higher.

Equation of state calculations of the volume change on mixing for these fluid pairs and compositional simulations of the Taylor dispersion experiment are given in Chapter 2.

1.2.3. ENHANCED DISPERSION EFFECTS IN MISCIBLE DISPLACEMENTS

The observed high mass transfer effects in the visual and Taylor dispersion experiments described above could have a significant impact on displacement behavior in miscible processes. The very high dispersion coefficients calculated above would most likely hold only for the initial contact between the oil and solvent, when the concentration gradients are the steepest and the largest negative volume change on mixing would be taking place. As the non-ideal mixing effects diminish, the mass transfer rates would reduce to those resulting from normal diffusion and dispersion. The initial rates are high

enough, however, that even if they were in effect for a short period of time, their effect could be significant.

Recovery of oil trapped by capillary forces or in dead-end pores by solvent flooding could be improved if enhanced dispersion effects were present. Large volume change on mixing when the solvent initially contacts an isolated oil droplet could lead to rapid mobilization of the oil. Solvent override caused by gravity segregation would be decreased by rapid initial mass transfer rates on contact with the oil and the degree of fingering in unstable displacements could be reduced. Large levels of dispersion could stabilize displacements even with highly unfavorable mobility ratios, eliminating unstable frontal advance and creating higher initial oil recoveries.

Conventionally recognized dispersion mechanisms: molecular diffusion, microscopic convective dispersion and macroscopic dispersion, and unstable displacement effects such as gravity override and viscous fingering, have been shown to play important roles in miscible displacement processes (e.g. Stalkup, 1983). The enhanced dispersion effect due to non-ideal mixing that was observed in the Shell Canada experiments could potentially have a very great effect on these processes as well. It also illustrates the possible importance of phase behavior models capable of describing the volume change on mixing of oil solvent.

1.3. TREATMENT OF DISPERSION AND VISCOUS FINGERING IN MISCIBLE DISPLACEMENT RESERVOIR SIMULATION

As shown by the above review, a generally applicable simulator for modeling miscible displacements must describe a variety of physical processes. Phase behavior models may require multiphase equilibria, component partitioning between phases and non-ideal mixing calculations. Flow calculations may include compressible flow, dispersion

due to any of the processes described above, and treatment of unstable frontal advance. Several surveys of the methods used for miscible displacement simulation are available in the literature, for example: Ewing (1988), Fayers (1987), Russell and Wheeler (1983), and Young (1984).

Currently, the vast majority of simulators assume complete and instantaneous mixing of fluids within each reservoir grid block, with one exception being the incomplete mixing compositional simulator presented by Nghiem et al. (1989). Non-ideal mixing and transport property variations are only accounted for by inter-block variations; thus the resolution of the simulation is limited by the number of grid blocks used. If the displacement of oil in the enhanced recovery process is stable, the complete-mixing assumption is valid, as the displacing front is well defined and the oil in place and injected gas will be well mixed at the front. In both miscible and immiscible gas injection processes, however, frontal advance is often unstable.

In modeling unstable frontal advance, the scale of the fingers is usually much smaller than the size of a grid-block used in a typical field scale reservoir simulation. Explicit modeling of viscous fingers is possible with fine-grid simulation of laboratory scale displacements; Kempers (1991), for instance, presents experimental and fine-grid simulation results showing generation of a dispersive mixing zone in both stable and unstable miscible displacements. Since fine-grid simulation of field scale processes is impossible, due to computational limits, those simulators that attempt to describe unstable frontal advance generally use lumped parameter approaches which describe the essential characteristics of miscible displacement without reproducing the fine structure of the viscous fingers.

A discussion of stability and numerical dispersion problems, of particular importance for miscible displacement modeling, and a brief review of the techniques used in both modified black-oil and compositional simulation of miscible processes is given below.

1.3.1. STABILITY AND NUMERICAL DISPERSION

It has been shown (Peaceman, 1977) that the solution of the discretized convection equation is equivalent to an exact solution of the convection-diffusion equation, with a diffusion coefficient dependent on grid block and time step sizes. This artificial dispersion term is caused by truncation of the Taylor series in the discretization scheme, and is often denoted as "numerical dispersion" (e.g. Aziz and Settari, 1979; p. 335). Solution of the discretized convection-diffusion equation is equivalent to an exact solution of the convection-diffusion equation, with the diffusion coefficient given by the sum of the physical diffusion and numerical dispersion. The exact magnitude of the numerical dispersion depends on the type of discretization, as well as the size of the grid blocks and time steps.

Stability of an algorithm implies that errors introduced at one stage of the computation are not amplified by further computation (Aziz and Settari, 1979; p. 58). Stability and numerical dispersion are closely connected in that numerical dispersion acts to stabilize the difference equation. The discretization scheme commonly in use for reservoir simulation is backward-in-distance (upstream weighting) and either backward-in-time (implicit) or forward-in-time (explicit). Explicit formulations generally exhibit less numerical dispersion, but have a time step limit imposed by stability considerations for a given size of grid block, while implicit methods show much higher numerical dispersion. Models which use implicit pressure and explicit saturation and composition (IMPES)

formulations are a popular compromise between fully explicit or implicit models. IMPES models are subject to the "throughput" stability condition, which requires that no more than one pore volume of material may be put through a grid block in one time step. Peaceman (1977) presents a thorough discussion of stability and numerical dispersion for various weighting schemes.

A related problem is the grid orientation effect. When simulating an element of a well pattern in the field, injection and production wells can be at opposite corners of a square grid pattern (diagonal grid) or at opposite ends of a single side of the grid (parallel grid). These two grids can give different solutions to a given problem; the finite difference solution converges to two different results as the grid is refined for the two orientations. The effect is most severe for highly unfavorable mobility ratio displacements, however, the presence of dispersive forces tends to decrease the orientation error (Aziz and Settari, 1979; p. 334).

Todd et al. (1972) proposed two-point upstream weighting of the relative permeabilities, which reduced both numerical dispersion and grid orientation effects for mobility ratios in the range of 1 to 10. Similar to this approach, Vinsome and Au (1979) suggest harmonic weighting of upstream mobilities. Yanosik and McCracken (1979) presented a nine-point discretization method for areal displacements, as opposed to the standard five-point scheme, which essentially eliminated the grid orientation effect for mobility ratios up to 50, however, nonphysical distortion of displacement fronts may also result with this method.

Other higher order discretizations of the flow equations have been proposed, for example by Bell and Shubin (1985) and Shiralkar and Stephenson (1991). Very good results have been obtained for control of numerical dispersion and the grid orientation

effect, however, application of these schemes can result in oscillations in the solution unless sufficient dispersive forces exist. Research on these methods has been directed towards eliminating these oscillations.

1.3.2. MODIFIED BLACK-OIL MODELS

Over three quarters of reservoir simulation studies may be performed using black-oil models (Mattax and Dalton, 1990). These simulators model immiscible flow with fluid properties treated as functions of pressure only or as functions of pressure and solution gas/oil ratio. The existence of a maximum of three distinct phases is assumed: aqueous, heavy hydrocarbon and light hydrocarbon. The governing equations for the model are derived from mass conservation equations on three components: water, oil and gas, with the gas component existing in both the heavy hydrocarbon and light hydrocarbon phases. The miscible displacement simulators discussed in this section are termed modified black-oil models as they all use two or three components and restrict the number of hydrocarbon phases to one or two.

Peaceman and Rachford (1962) presented a model which accounted for dispersion by using the convection-dispersion equation for mass conservation. The model is developed with the following assumptions: (a) two components, oil and solvent, are present in a single phase (complete miscibility); (b) flow is incompressible; (c) mixing is ideal. The dispersion tensor includes constant longitudinal and transverse dispersion terms. The model equations are discretized using a combination of centered-in-distance and backward-in-distance with centered-in-time differences. This hybrid is used to try and minimize numerical dispersion and oscillations in the solution. The difference equations are solved using a sequential implicit technique. In two-dimensional simulations of adverse

mobility ratio displacements, fingering effects were observed due to the input permeability distribution which were similar to those observed experimentally.

Chaudhari (1971), Russell and Wheeler (1983), and Young (1984) have all investigated solutions of the system of equations proposed by Peaceman and Rachford. A number of higher order discretization schemes, primarily using the sequential implicit solution method were used. In some cases, negative artificial dispersion was employed to eliminate oscillations. Numerical dispersion and grid orientation effect were minimized by selecting the best discretization method for a given physical problem. These models have not been widely used, in part due to the perception that the convective-dispersion equation will over-predict oil recovery unless viscous fingers are explicitly modeled. Young (1986) presents evidence that this assertion is unfounded.

Lantz (1970) described modifications to a two-phase black-oil simulator to allow the modeling of two component (oil and solvent) miscible displacements. The flow equation considering convection only was used for continuity and incompressible flow and ideal mixing was again assumed. An exact analogy between the equations for immiscible and miscible flow was developed in which bulk immiscible flow becomes bulk miscible flow and flow due to capillary forces became diffusive flux. Velocity dependent convective dispersion was not modeled. Backward-difference and central-difference implicit and explicit formulations were studied. The most severe limitation of the simulator was found to be numerical dispersion.

The original attempt to account for the effects of viscous fingering without simulating the growth of individual fingers is due to Koval (1963). The treatment was analogous to the Buckley-Leverett equations for frontal advance and fractional flow in immiscible displacements. The effect of fingering was accounted for in a fully miscible,

two component model by employing an effective viscosity ratio to alter the fractional flow of solvent (volume fraction of solvent flowing). The fractional flow of solvent was defined as the ratio of the solvent mobility to the total mobility:

$$f_s = \frac{k_{rs}/\mu_s}{k_{ro}/\mu_o + k_{rs}/\mu_s} \quad (1.8)$$

Under miscible conditions, $k_{rj} = S_j$ ($j=o,s$), giving

$$f_s = \frac{1}{1 + \frac{\mu_s}{\mu_o} \frac{S_o}{S_s}} \quad (1.9)$$

Koval varied the solvent/oil viscosity ratio in the above equation by letting the oil viscosity remain unaltered, and replacing the solvent viscosity with an effective viscosity defined as follows:

$$\mu_{se} = [S'_s \mu_s^{-1/4} + S'_o \mu_o^{-1/4}]^{-4} \quad (1.10)$$

where S'_s is an adjustable parameter used to fit experimental data. Koval found good agreement to the experimental data of Blackwell et al. (1959), with the following:

$$S'_s = 0.22, \quad S'_o = 1 - S'_s = 0.78 \quad (1.11)$$

Another fractional flow alteration technique was proposed by Todd and Longstaff (1972). They apply their method to a fully miscible, two hydrocarbon component model based on the convection equation without diffusion. The viscosity terms shown in equation (1.9) are replaced with effective viscosities as follows:

$$\begin{aligned} \mu_{se} &= \mu_s^{1-\omega} \mu_m^\omega \\ \mu_{oe} &= \mu_o^{1-\omega} \mu_m^\omega \\ \mu_m &= [S_s \mu_s^{-1/4} + S_o \mu_o^{-1/4}]^{-4} \end{aligned} \quad (1.12)$$

In this formulation, ω is a mixing parameter that may be adjusted to match experimental data. A value of $\omega=0$ implies segregated flow, while a value of $\omega=1$ corresponds to complete mixing. Todd and Longstaff recommend values in the range of $\omega=1/3$ to $2/3$.

Fayers (1988), and Fayers and Newley (1988) present another model for fractional flow alteration, incorporating an empirical relation for the finger volume fraction. They define the conservation equation for solvent, with a finger volume fraction S_f and concentration of solvent in the finger C_s , as follows:

$$\phi \frac{\partial(S_f C_s)}{\partial t} + q \frac{\partial(f_f C_s)}{\partial x} = 0 \quad (1.13)$$

where the fractional flow of the finger is given by

$$f_f = \frac{S_f / \mu_f}{S_o / \mu_o + S_f / \mu_f} \quad (1.14)$$

The finger viscosity is evaluated using a one quarter power mixing rule as in the Koval or Todd and Longstaff models. In this case the viscosity alteration applies only to the finger:

$$\mu_f = [C_s \mu_s^{-1/4} + (1 - C_s) \mu_o^{-1/4}]^{-4} \quad (1.15)$$

The empirical relation for finger volume fraction is given as

$$S_f = a + b C_s^\alpha \quad (1.16)$$

where the parameters a and b are constant:

$$a = 0.1, \quad b = 1 - a = 0.9 \quad (1.17)$$

and the parameter α is correlated to the mobility ratio to fit experimental data. The following form was found to fit the data of Blackwell et al. (1959):

$$\alpha = 0.42 (\mu_o / \mu_s)^{0.4} \quad (1.18)$$

The advantage of the Fayers model over the other fractional flow alteration models is that the basic physical approximations can be translated consistently to three dimensions,

maintaining the vectorial nature of the fingering phenomenon, thus giving more dependable results in field applications.

1.3.3. COMPOSITIONAL MODELS

In general, two classes of problems requiring compositional treatment can be identified (Coats, 1980). The first type includes depletion or cycling of volatile oil and gas condensate reservoirs. The second type includes enhanced oil recovery processes such as gas miscible flooding with multi-contact miscibility generated in situ. In both of these cases, large compositional variations in the phases can exist as a result of phase changes and mass transfer between phases. One distinction between these types of problems is that the first class usually involves phase compositions far removed from the critical point, while the second class generally requires calculation of phase compositions and properties in the near-critical region. The use of compositional simulation models is especially advantageous for this second class of problem, as the equation of state thermodynamic model provides a single, consistent source of equilibrium K-values and phase densities for all phases even in the critical region.

Equation of state compositional simulators generally assume complete and instantaneous mixing within grid blocks and negligible dispersion, but do not assume incompressible flow or ideal mixing. Fussell and Fussell (1979) presented a compositional model using an equation of state for both phase equilibria and density calculations, as opposed to table lookup for equilibrium ratios. The model equations were developed by writing molar balances for each hydrocarbon component, assuming complete mixing and negligible dispersion. The total hydrocarbon mole balance, water mole balance, phase equilibria relations and sum of mole fraction constraints complete the model. An IMPES type solution scheme was used, and the flow and phase equilibria equations were solved

simultaneously using a technique to minimize the number of variables for which simultaneous iteration is required. Newton-Raphson iteration was used to correct the iteration variables. Physical dispersion was not taken into account, and no method for control of numerical dispersion was used.

The same set of model equations has been treated using a variety of solution methods. Young and Stephenson (1983) presented an IMPES type model, while Coats (1980) used a fully implicit method and solved the full set of equations simultaneously; both use Newton-Raphson iteration to update the iteration variables. Coats used a simple form of numerical dispersion control by specifying that the composition of oil flowing out of a grid block will be the original oil composition until a gas phase forms in that block. Chien et al. (1985) also used a fully implicit formulation with Newton-Raphson iteration. Equilibrium K -values were used, instead of mole fractions, along with pressure and overall concentrations as the iteration variables. No numerical dispersion control was implemented.

Nghiem et al. (1981) proposed an IMPES formulation, combined with a successive substitution algorithm which separates the solution of the flow and thermodynamic calculations, allowing a powerful flash algorithm to be used for the phase equilibria calculations. Numerical dispersion control was obtained through two-point upstream weighting of the compositions in the coefficients of the flow equation.

Chase and Todd (1984) developed a model based on component mole balances which handled viscous fingering with a mixing parameter formulation like those used in the black-oil models, however table-lookup was used for equilibrium ratios, not equation of state calculation. A Runge-Kutta algorithm was used for solution of the equations, and truncation error was limited simply by choosing the maximum possible time step size.

Acs et al. (1985) derived the pressure equation from a volume balance, rather than as a sum of the mole balances. The equations were solved using an IMPES technique, with K -values and liquid densities input as tables of experimental values, and only the gas phase density calculated from an equation of state. For this model, dispersion was handled by using the full convection-diffusion equation, requiring a dispersion tensor for each component. Watts (1986) also used the volume-balance approach for the pressure equation. However, he neglected dispersion in the formulation and solved the equations using a sequential implicit technique. Iteration variable updating in both these models was through successive substitution.

Collins et al. (1986) presented an adaptive-implicit model which solved the equations implicitly only for the grid blocks in which the iteration variables were changing rapidly. An IMPES solution technique was used for the other blocks. Dispersion was neglected in the flow equations, which were solved using Newton's method. The equation of state flash calculations were decoupled from the flow equations, allowing the use of a robust flash algorithm. Again, no numerical dispersion control measures were given.

More recently, compositional simulators based on the full convective-diffusion equation have been developed. These are characterized by the use of higher order discretization schemes used to limit numerical dispersion so that the effect of physical dispersion present in the model can be seen. Young (1986) presented a model in which the dispersion coefficient equation included a viscosity gradient term to increase the size of the mixing zone which is characteristic of unstable displacements. The use of the convective-dispersion equation allows simulation of the stabilizing effect of dispersion on adverse mobility ratio displacements, which cannot be predicted by fractional flow alteration techniques. A third order discretization scheme was used by Young (1986) with negative artificial dispersion to eliminate oscillations.

Taggart and Pinczewski (1987) use the full convection-diffusion equation in the development of their model, however, ideal mixing and incompressible flow are assumed. Equilibrium phase compositions are obtained from an equation of state flash calculation. The model equations are discretized using a third order finite difference scheme and are solved via an IMPES approach. Flux corrected transport techniques are employed to eliminate oscillations. Chang et al. (1990) also use third order differencing on the full convection-diffusion equation, solving the resulting system with an IMPES scheme. In this formulation, the physical dissipative forces of capillary pressure and dispersion are relied upon to damp out oscillations in the solution.

The application of fractional flow alteration techniques to compositional simulation of multicomponent systems has received little attention in the literature. One approach is given by Crump (1988), extending the Todd and Longstaff model to a multiphase, multicomponent compositional simulator with simplified phase behavior predictions. Crump notes that, for multi-contact miscible processes, the mixing parameter model is inadequate due to the inconsistency between the complete mixing assumption for flash calculations and the partially segregated flow assumption for the calculation of fluid mobilities. The results of this paper, and the importance of the interaction between phase behavior and fingering phenomena as shown by Gardner and Ypma (1984) and Gardner et al. (1981), indicate the need for further research on compositional simulation models incorporating incomplete mixing at the grid block level.

One novel approach for modeling incomplete mixing with application to simulation of unstable displacements has been presented by Nghiem et al. (1989). This method distinguishes two flow regions in each reservoir grid block: a region where complete mixing occurs between the oil in place and the injected gas, and a bypassed region where the oil is not contacted by gas but can still flow under the influence of pressure gradients.

Transfer of components is allowed from the bypassed region, which is assumed to maintain constant composition, to the mixed region to simulate the mixing of injected fluid and original oil which takes place at the edges of the fingers. The transfer rate is described by a two-parameter model. In the work described, one parameter was fixed at a constant value while the other was fitted to experimental data. The bypassed oil is treated as a single pseudo-component, while equation of state flash calculations on the full multicomponent mixture are used to predict the phase behavior in the mixed region. Preliminary studies with this model have shown good agreement with experimental and fine-grid simulation data, and show superior performance over the Koval model.

1.4. PROPOSAL FOR TREATMENT OF DISPERSION IN COMPOSITIONAL RESERVOIR SIMULATORS

This dissertation investigates application of dispersion models for miscible displacement simulation. Physical dispersion due to molecular diffusion, microscopic convective dispersion, macroscopic dispersion or enhanced dispersion due to non-ideal mixing may all be present to some degree in a given miscible displacement system. As was shown in the review of physical processes, all of these dispersive forces may be described by an effective dispersion coefficient. Viscous fingering due to unfavorable mobility ratios will be present in many miscible displacements. The effect of this unstable frontal advance on recoveries may also be described with dispersion relationships (Young, 1986).

In order to correctly model non-ideal mixing effects, a compositional equation of state simulator is required. As discussed above, dispersion in equation of state compositional simulation has been treated by applying the full convective-dispersion equation. Mixing parameter models have been applied primarily to black-oil models or compositional models with simplified phase behavior descriptions.

As many compositional simulators with sophisticated phase behavior modeling and varying degrees of numerical dispersion control have been developed based on discretization of the convection equation without dispersion, the approach to dispersion modeling taken in this work is to develop models which could be implemented within the framework of one of these conventional compositional simulators. An IMPES formulation of the compositional model equations with a provision for two-point upstream weighting will be used as the base to which dispersion models will be added. The use of these models to describe dispersion and incomplete mixing present in unstable displacement at scales smaller than those of a typical field scale grid block is of primary importance. Minimization of numerical dispersion while describing physical dispersion is also addressed. Higher order discretization schemes have not been investigated in this work, however, the models developed here would be applicable to simulators using these methods.

Several works on modeling dispersion/incomplete mixing in compositional simulation without use of the full convective-dispersion equation have been reported. The incomplete mixing compositional model proposed by Nghiem et al. (1989) was used by Ammer et al. (1991) to model a carbon dioxide miscible displacement in which volume change on mixing was significant. They report that this simulator was capable of matching experimental results with one fitted parameter; black-oil, pseudo-miscible and conventional compositional simulators were found to give less accurate matches. Barker and Fayers (1991) develop transport coefficients which alter the compositions of fluids flowing out of a large grid block in relation to the average compositions of those fluids within the grid block. The values of the coefficients are calculated from fine grid simulations of heterogeneous media.

Diffusion effects have been added to a conventional compositional simulator by Thiebot and Sakthikumar (1991). In this work, Fick's first law is used to predict diffusive flux across grid block boundaries, which is then added as source or sink terms in the convective flow equation. Hu et al. (1991) present a model of a laboratory core experiment in which diffusion from the core into a fracture (open space) is modeled with an analytical solution of the convective-diffusion equation and flow within the core itself is handled with a standard compositional formulation.

The impetus for the approach to dispersion modeling investigated in this work comes from recent developments in pressure transient analysis, utilizing semi-analytical techniques for solution of the pressure diffusion equation. A brief discussion of these methods is given next, followed by the proposal to incorporate these solutions for dispersion modeling in compositional simulation.

1.4.1. USE OF SEMI-ANALYTICAL MODELS IN PRESSURE TRANSIENT ANALYSIS

van Everdingen and Hurst (1949) first applied the method of Laplace transforms for solution of the pressure diffusion equation for flow problems in reservoirs. Gringarten and Ramey (1973) investigated potential flow with the use of Green's function theory for solution of the diffusion equation, in which the differential equation is recast into integral form. Following this approach, Cinco-Ley et al. (1978) derived the integral equation formulation for the transient flow problem for a hydraulically fractured reservoir. The resulting solution is an integral equation in which the boundary conditions are taken into account implicitly. The integration was then performed numerically. This formulation is known as the Boundary Integral Equation Method or Boundary Element Method (BEM). van Kruijsdijk (1988) combines the technique of Cinco-Ley et al. with the Laplace

transform to obtain a considerable simplification in the formulation. The numerical Laplace inversion algorithm given by Stehfest (1970) was used by van Kruijsdijk to generate the time domain solutions. Kikani and Horne (1989) use BEM with the pressure diffusion equation to solve a number of general reservoir problems including streamline generation and front tracking for steady state cases as well as application to pressure transient testing of arbitrarily shaped, multi-well multi-rate reservoirs.

Boundary Integral Equation Methods for solution of linear differential equations will reduce the dimensionality of the problem by one; i.e., a three-dimensional problem reduces to a surface integral, while a two-dimensional problem reduces to a contour integral. The fact that it is an integral method, which is a smoothing procedure, eliminates the truncation error and grid orientation effect inherent in discretization methods for solution of differential equations.

1.4.2. PROPOSED INVESTIGATION OF ANALYTICAL AND SEMI-ANALYTICAL MODELS FOR TREATMENT OF DISPERSION IN COMPOSITIONAL SIMULATORS

A multicomponent, two hydrocarbon phase compositional simulator with component conservation described by the convective flow equation is developed as the base model. Phase fractions, densities, and equilibrium ratios are given by a cubic equation of state.

Evaluation of diffusive flux from Fick's first law and from solutions of Fick's second law (i.e., the diffusion equation) is considered. The solution of the diffusion equation using Green's function theory for prescribed flux boundary conditions and for zero order or first order linear initial conditions is described. Analytical solutions and

semi-analytical solutions (i.e., those requiring numerical inversion from the Laplace domain) are derived.

Application of Fick's first law to calculation of dispersive flux across grid block boundaries in the compositional simulator is considered first. Implementation of the solutions of the diffusion equation with various boundary and initial conditions for evaluation of dispersive flux within grid blocks and across grid block boundaries is then discussed. Use of these models for simulation of the Shell Canada visual experiment, Taylor dispersion experiment and a one-dimensional laboratory scale miscible displacement are given, and extension of the method to two dimensions is also discussed.

2. CONVENTIONAL COMPOSITIONAL SIMULATION OF TAYLOR DISPERSION EXPERIMENTS

Some experiments that demonstrate dispersion in miscible displacement operations were described in Section 1.2 of the previous Chapter. The results of the experiments (which were conducted by Laurie Sibbald and co-workers at the Shell Canada Calgary Research Center) were made available for analysis in this dissertation.

The experiments were of two types. In the first type of experiment (the "visual experiments" that were described in Section 1.2.1) the mixing took place without any external pressure gradients. The second type of experiment (the "Taylor dispersion experiments" described in Section 1.2.2) involved displacement of a slug of live oil (or a model hydrocarbon) held in a capillary tube with a solvent at a fixed solvent flow rate.

Shell Canada provided access to the equation of state compositional simulator (EOSIM) developed at the Bellaire Research Center of the Shell Development Company. This simulator has been used in modeling the Taylor dispersion experiments. (Because of the absence of any external driving forces and since dispersion is not included explicitly in the model, the simulator cannot be used to describe the visual experiments.)

The oil used in the study was a live oil from the Virginia Hills reservoir. The phase behavior model for the reservoir oil and the solvents is given first, followed by the simulation of the Taylor dispersion experiments.

2.1. PHASE BEHAVIOR OF MISCIBLE SOLVENTS AND RESERVOIR OIL

The phase behavior of the fluids examined in this work will be described by the Peng-Robinson equation of state. A five component characterization for the reservoir oil will be used with component compositions as given in Table 2.1 below.

Table 2.1: Reservoir Oil Component Characterization

Component	Mole Fraction
Methane	0.2608
Ethane	0.1044
I-Butane	0.1837
Hypothetical - H1H2	0.3153
Hypothetical - H3H4	0.1358

The properties for the above pure components and others used in this work are given in Table 2.2.

Table 2.2: Pure Component Properties

Component	Molecular Weight	Critical Pressure (kPa)	Critical Temperature (K)	Acentric Factor	Critical Volume (cm ³ /mol)
Methane	16.04	4594.60	190.53	0.0110	98.97
Ethane	30.07	4878.70	305.42	0.0990	147.94
Propane	44.10	4249.50	369.82	0.1540	202.86
I-Butane	58.12	3648.40	408.14	0.1840	262.70
N-Hexane	86.18	3032.20	507.90	0.2980	370.57
N-Octane	114.23	2488.10	568.81	0.3980	491.19
H1H2	137.00	2358.67	597.49	0.4596	526.51
H3H4	352.90	1103.61	809.50	0.9811	1524.58

All of the equation of state calculations performed in this work were done with all binary interaction parameters set to zero. Tuned parameters for fitting the oil two-phase boundary with the Peng-Robinson equation of state were not available, and the equation provided adequate representation of the molar volumes of the oil/solvent mixtures which are of importance in this study. The phase envelope for the reservoir oil, calculated using the two-phase boundary program of Michelsen (1990) with the Peng-Robinson equation of state, and the location of the critical points for some of the light hydrocarbons used as miscible solvents for this oil are shown below in Figure 2.1. Clearly, the reservoir pressure

and temperature of 22.75 MPa and 372 K represent conditions well into the supercritical region for these fluids.

As discussed in Chapter 1, the amount of volume change on mixing of oil and solvent is thought to affect the degree of enhanced dispersion present in a system. Calculations at constant pressure and temperature using the Peng Robinson equation of state were carried out on mixtures of oil and solvent with the volume fraction of solvent varying from 0 to 1. The results of these calculations are shown as a ratio of the volume of the mixture to the volume of the unmixed solvent and oil constituents. These results are shown in Figure 2.2 for ethane solvent with the reservoir oil, in Figure 2.3 for ethane solvent with oil represented simply by n-octane and in Figure 2.4 for the reservoir oil with a mixed solvent of methane and ethane. The calculations are carried out at the reservoir pressure of 22.75 MPa and temperatures of 98.9 °C and 20 °C. All systems show similar

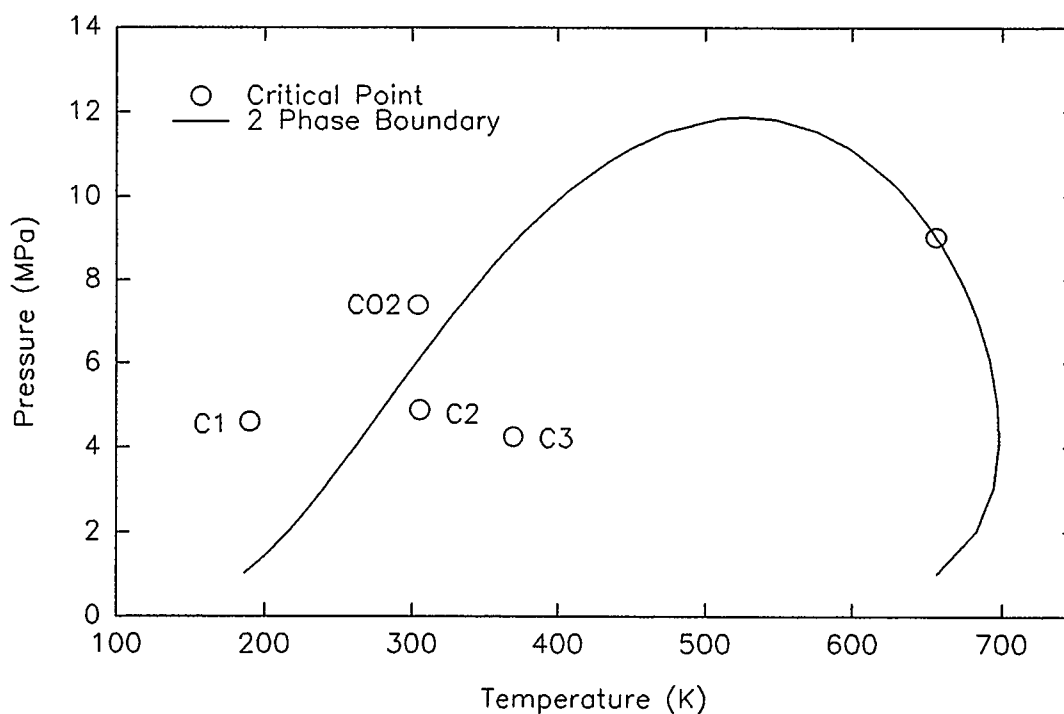


Figure 2.1: P-T Diagram for Reservoir Oil plus Solvent Critical Points

behavior, with the maximum volume change ranging from about 7% for ethane and oil to about 12% for the mixed solvent with oil. The ethane + n-octane system is used in this work as a simple two component model which exhibits approximately the same negative volume change on mixing present in the oil + ethane system.

The Taylor dispersion experiments were carried out for the ethane + oil system and for n-hexane solvent with n-octane solute. In both of these cases, the oil slug is completely miscible with the solvent drive fluid. Equation of state calculations on n-hexane + n-octane mixtures show a maximum negative volume change on mixing of less than 0.05%. The n-hexane plus n-octane runs were performed to provide experimental results for a system with negligible volume change, and therefore no enhanced dispersion effects.

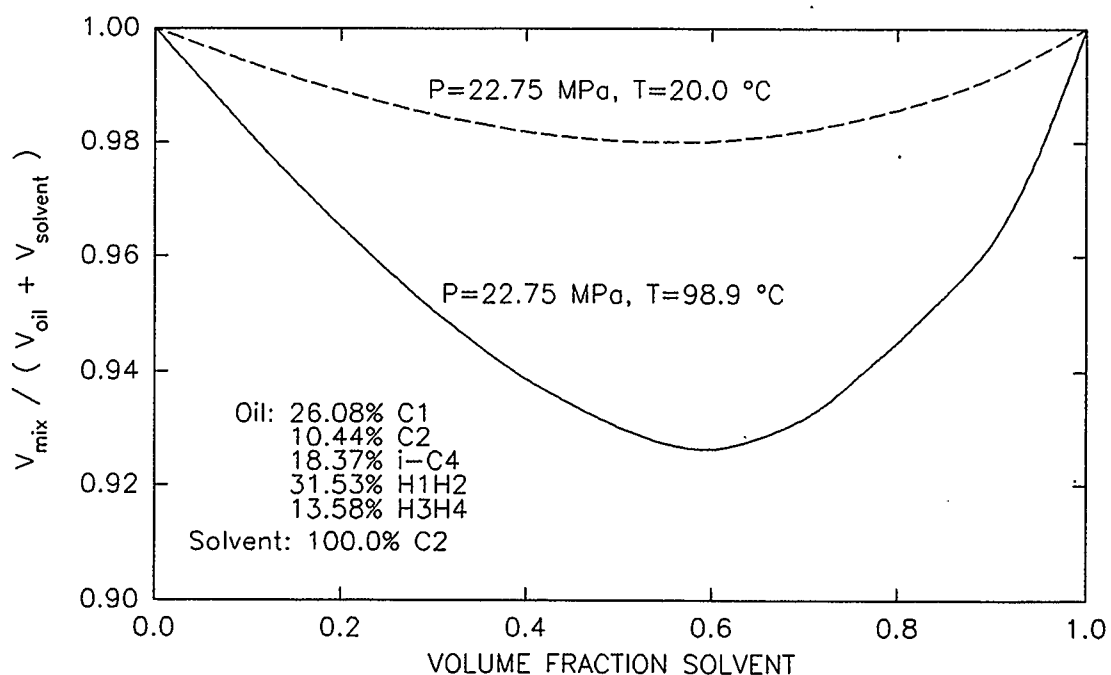


Figure 2.2: Volume Change on Mixing, Oil + Ethane

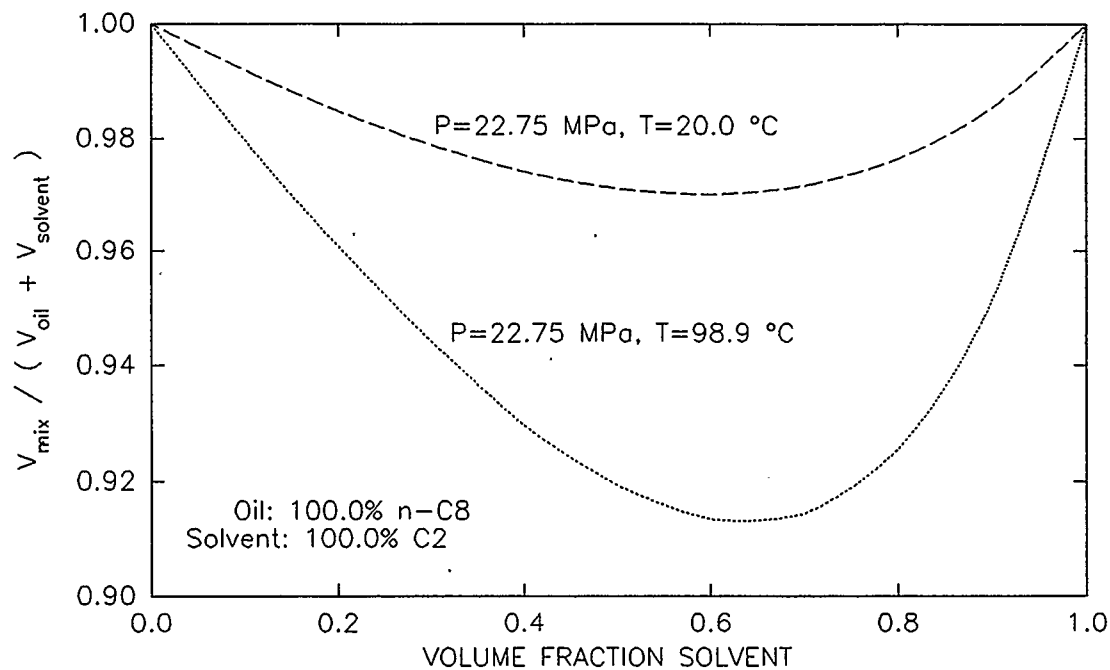


Figure 2.3: Volume Change on Mixing, n-Octane + Ethane

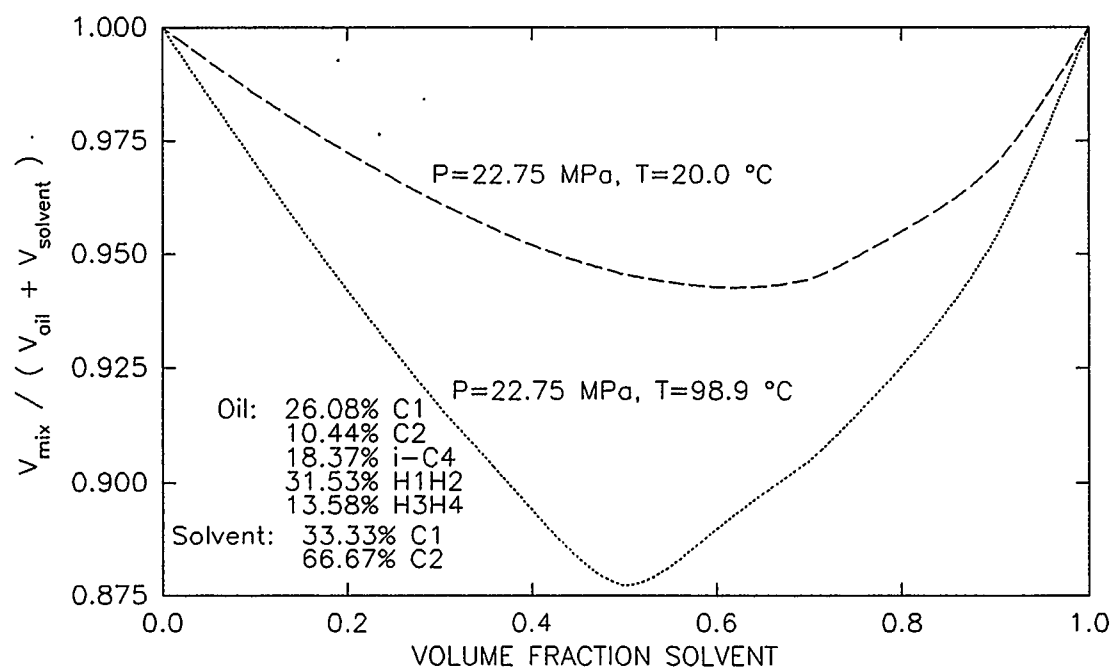


Figure 2.4: Volume Change on Mixing, Oil + Methane/Ethane

2.2. TAYLOR DISPERSION EXPERIMENT SIMULATION

2.2.1. MODEL DEFINITION

The EOSIM simulator is based on a discretization of the convective flow equation, with the option of using single-point or two-point upstream weighting of the component mobilities. Dispersion is not included explicitly in the model. However, as was discussed in Section 1.3.1 of Chapter 1, the solution of the discretized flow equation is equivalent to an exact solution of the convection-diffusion equation with a diffusion coefficient dependent on grid block and time step sizes (Peaceman, 1977). Also, numerical dispersion of this kind can be controlled by "upstream weighting" in addition to modifying the grid sizes (Aziz and Settari, 1979).

The Peng-Robinson equation of state is used to describe the phase behavior of the system, and the upstream weighting options and levels of grid refinement are varied in an attempt to match the experimental results.

The capillary tube has a circular cross-section with an area of $5.0 \times 10^{-3} \text{ cm}^2$. This is modeled as a one dimensional system with a square cross-section, 0.0707 cm on a side. For the open capillary tube, porosity is of course 100%. Permeability of the open tube is derived through a comparison of Darcy's law and the Hagen-Poiseuille equation for laminar flow in a tube; Reynolds numbers for the systems investigated are less than one, thus flow will be in the laminar regime. Darcy's Law for one-dimensional flow may be written as (Peaceman, 1977; p. 2):

$$\frac{Q}{A} = -\frac{k}{\mu} \frac{dP}{dx} \quad (2.1)$$

while the Hagen-Poiseuille equation is given by (McCabe and Smith, 1976; p. 89):

$$\frac{Q}{A} = -\frac{R^2}{8\mu} \frac{dP}{dx} \quad (2.2)$$

Equating these two forms results in the permeability being given by:

$$k = \frac{R^2}{8} \quad (2.3)$$

Evaluating R from the cross-sectional area of the circular tube gives a value for permeability of $k = 2.0 \times 10^4$ darcys. A constant solvent rate of 0.2 mL/hr is specified at the injector, and a constant back pressure is specified at the production end. Initially, the fluid in the tube is assumed to have a constant pressure everywhere equal to the back pressure constraint. The initial fluid distribution is shown below in Figure 2.5. The upstream solvent leg and the oil leg have initial lengths of 120.8 cm each, and the downstream solvent leg has an initial length of 619.1 cm.

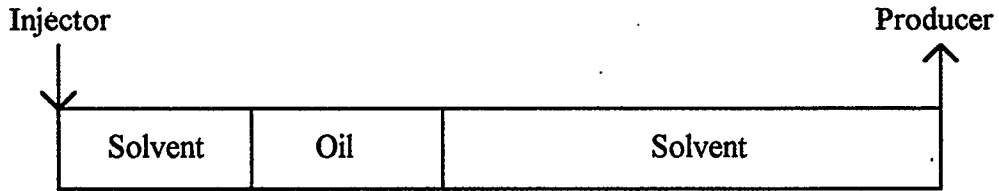


Figure 2.5: Taylor Dispersion Experiment Model Schematic

2.2.2. SIMULATION RESULTS

The first run of the Taylor dispersion experiment used the live oil described above with ethane solvent at a temperature of 98.9 °C and with a back pressure constraint of 22.75 MPa. Effluent composition data were obtained by taking samples of live fluid periodically and injecting them directly into a gas chromatograph column. The experimental data for this run are shown in Figure 2.6 (page 41).

The results obtained with the simulator using 114 grid blocks are shown in Figure 2.7 on the same page. The mole fractions of the two heavy hypothetical components are

lumped to compare to the experimental results for the C6+ mole fraction. In this case, the oil slug is assumed to occupy 16 grid blocks initially, resulting in a total of 114 grid blocks. Two-point upstream weighting of the mobilities is used, and the model is run to a termination time of 22.2 hr with a maximum time step size of 500 s. This weighting scheme and maximum time step size are used for all the runs described in this section, as the single point weighting scheme was found to require an excessive number of grid blocks to match the experimental results. A similar simulation run is shown in Figure 2.8 (page 42), for a 228 grid block model.

In these simulations, two-point upstream weighting is used to minimize the number of grid blocks required to model the experimental results. The inflection points present in the simulated effluent profiles are artifacts of the two-point scheme which arise in cases which exhibit large negative volume changes on mixing. As there is no method for describing physical dispersion in the simulator, the smearing of the fluid fronts in the model results is due solely to numerical dispersion. For a given time step size, the amount of numerical dispersion is proportional to the size of the grid blocks, as can be seen by comparing the results of the simulations with 114 and 228 grid blocks. For the ethane plus live oil run, the amount of physical dispersion is more closely mimicked by the higher numerical dispersion, coarse grid block simulation. Excluding the inflections mentioned above, the overall shape of the profiles and level of dispersion can be modeled correctly. The offset of the simulated results from the experimental ones is primarily due to the fact that the actual length of the initial downstream solvent segment cannot be matched with a whole number of grid blocks when the oil slug is defined with a whole number of grid blocks.

The first simulation run using 114 grid blocks for the n-hexane plus n-octane system is shown in Figure 2.9 (page 42). The experimental results are shown in Figure

2.10 (page 43) and the simulated results obtained with 228 grid blocks are shown in Figure 2.11 on the same page. The experimental results for the n-hexane plus n-octane run are more closely modeled by the fine grid, low numerical dispersion simulation. The simulations in this case also do not show any of the non-physical inflections present in the previous examples.

The final two sets of simulation results for the Taylor dispersion experiments are shown in Figures 2.12 and 2.13 (page 44); these figures show the results of the 114 grid block simulation for ethane solvent plus n-octane slug, at 20 °C (low volume change on mixing) and at 98.9 °C (high volume change on mixing) respectively. The 20 °C case is very similar to the n-hexane plus n-octane 114 grid block run, with the ethane/n-octane results showing the effects of slightly greater shrinkage. The 98.9 °C case shows the effects of even larger shrinkage, and also the appearance of the non-physical inflections caused by the interaction of the two-point upstream weighting scheme with the higher volume change on mixing. These results are shown here as the ethane plus n-octane system is used as a model system for testing the dispersion models developed in this work due to the similarities between this system and the ethane plus live oil system.

The experimental results and the results of the simulations show that an enhancement to dispersion occurs for the ethane plus live oil case with high volume change on mixing, over the level of dispersion present for the n-hexane plus n-octane run with essentially no volume change on mixing. This illustrates the need to accurately predict this volume change on mixing, as well as treat physical dispersion in the simulation of processes involving fluids of this nature.

2.3. SUMMARY

The results of the simulations show that it is possible to mimic the dispersive effect by choosing the appropriate level of grid refinement with a conventional compositional simulator. Expressions for calculating the coefficient of numerical dispersion have been developed for certain simplified cases (Mattax and Dalton, 1990; p. 60). The coefficients are found to be functions of the grid block and time step sizes, the velocity of the fluid and the derivatives of the fractional flow curves with respect to phase saturation. In practical reservoir simulation problems these quantities can vary considerably, making exact calculation of the coefficient of numerical dispersion impossible. Thus accurate predictive simulations using numerical dispersion to model physical dispersion can not be performed with a conventional compositional simulator. Also, this simulator cannot handle situations such as those present in the visual experiment in which no externally applied gradients are present for the system.

Developing a compositional simulator capable of accurately describing the phase behavior of fluids in miscible processes, and describing mixing via dispersion, which can be used for predictive simulation of processes with significant dispersion is the purpose of this work.

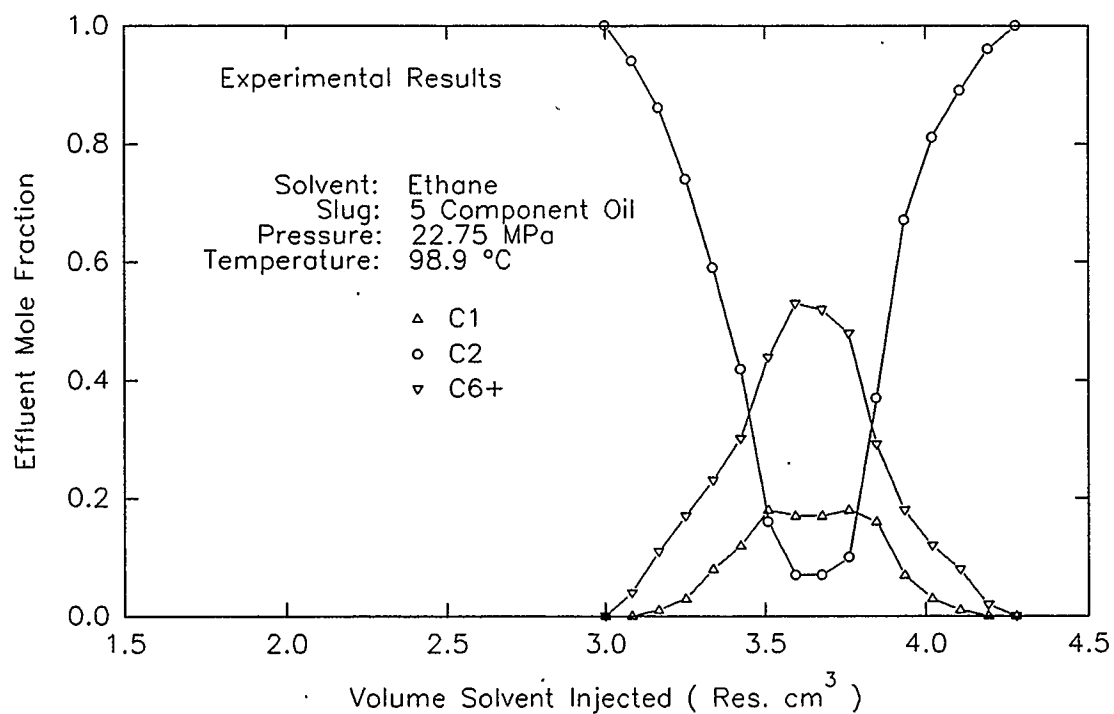


Figure 2.6: Taylor Dispersion Experiment - Ethane plus 5 Component Oil, Experimental Results

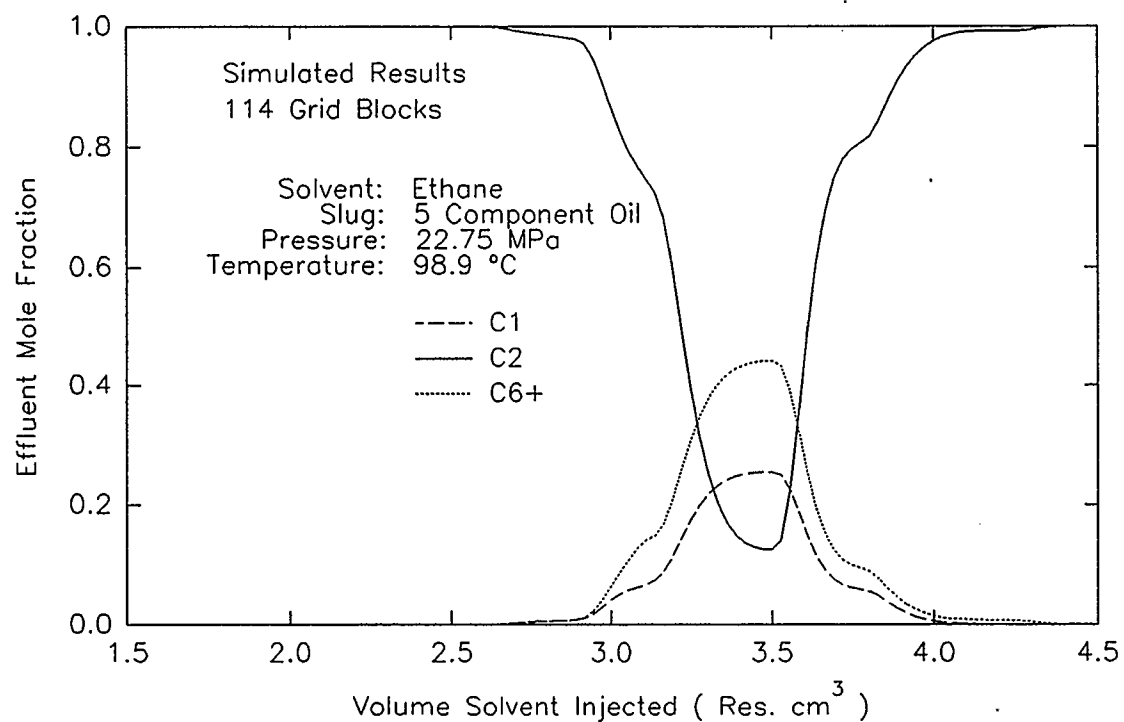


Figure 2.7: Taylor Dispersion Experiment - Ethane plus 5 Component Oil, 114 Grid Blocks

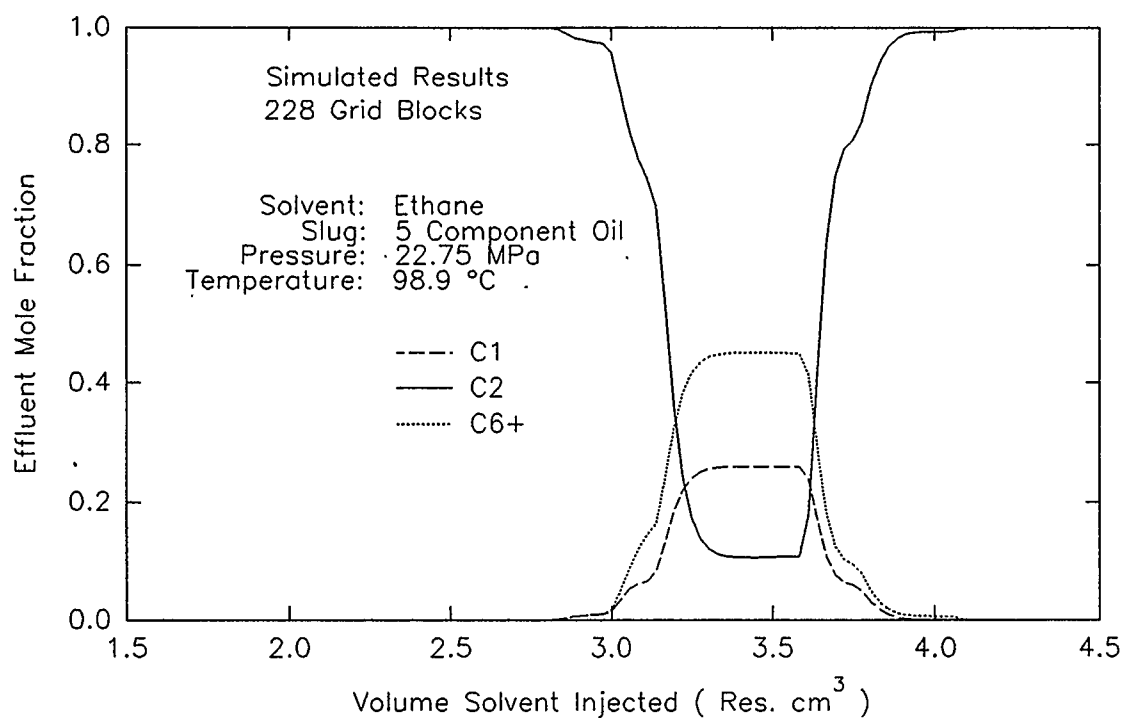


Figure 2.8: Taylor Dispersion Experiment - Ethane plus 5 Component Oil, 228 Grid Blocks

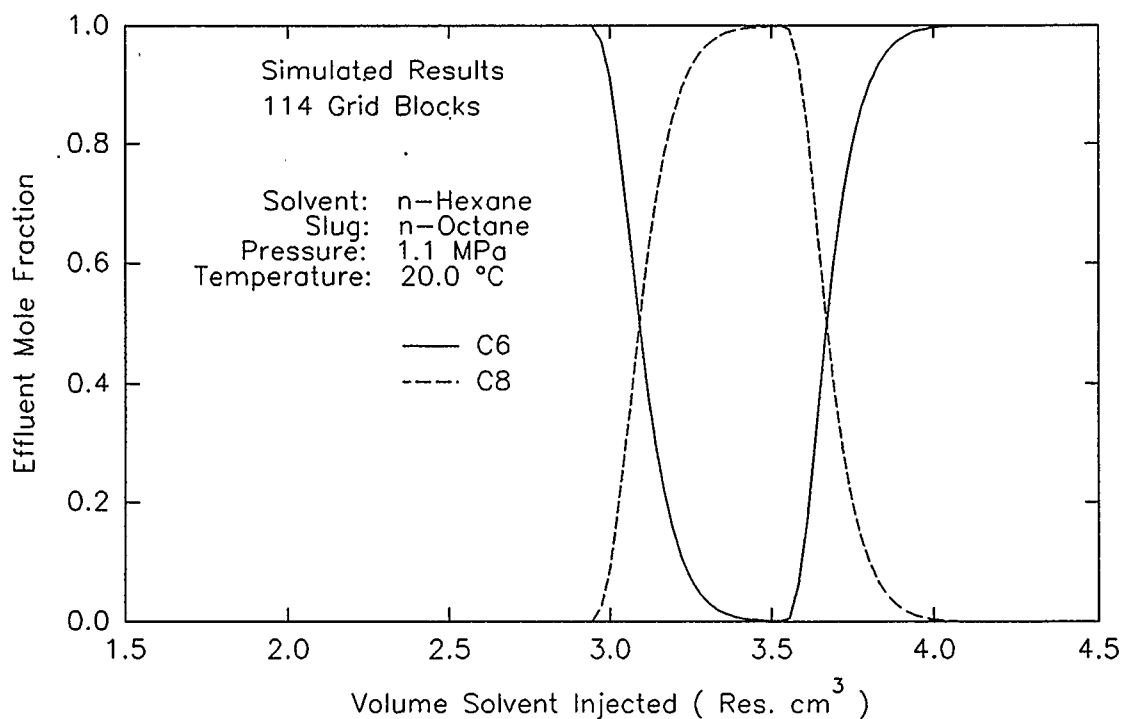


Figure 2.9: Taylor Dispersion Experiment - n-Hexane plus n-Octane, 114 Grid Blocks

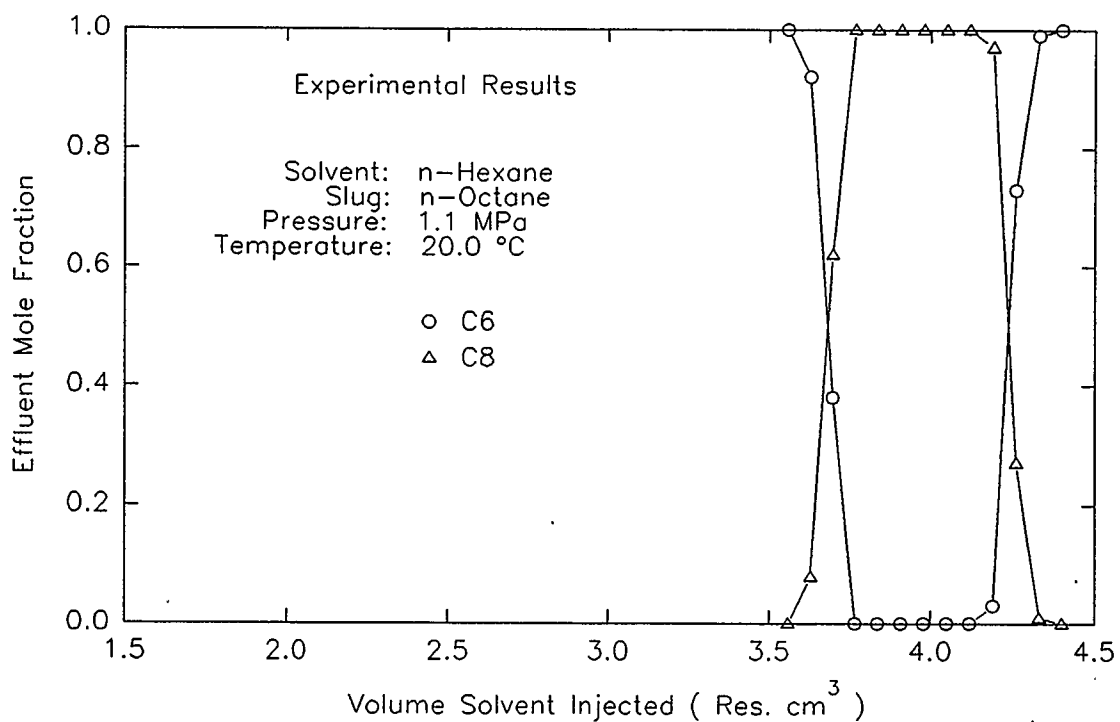


Figure 2.10: Taylor Dispersion Experiment - n-Hexane plus n-Octane, Experimental Results

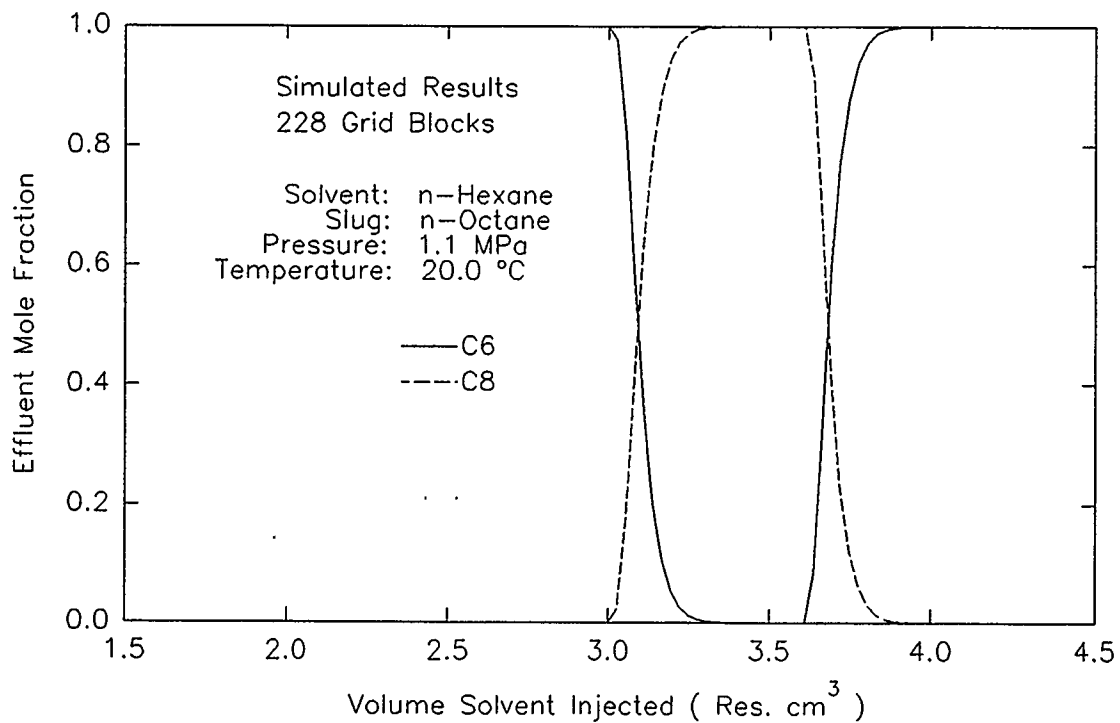


Figure 2.11: Taylor Dispersion Experiment - n-Hexane plus n-Octane, 228 Grid Blocks

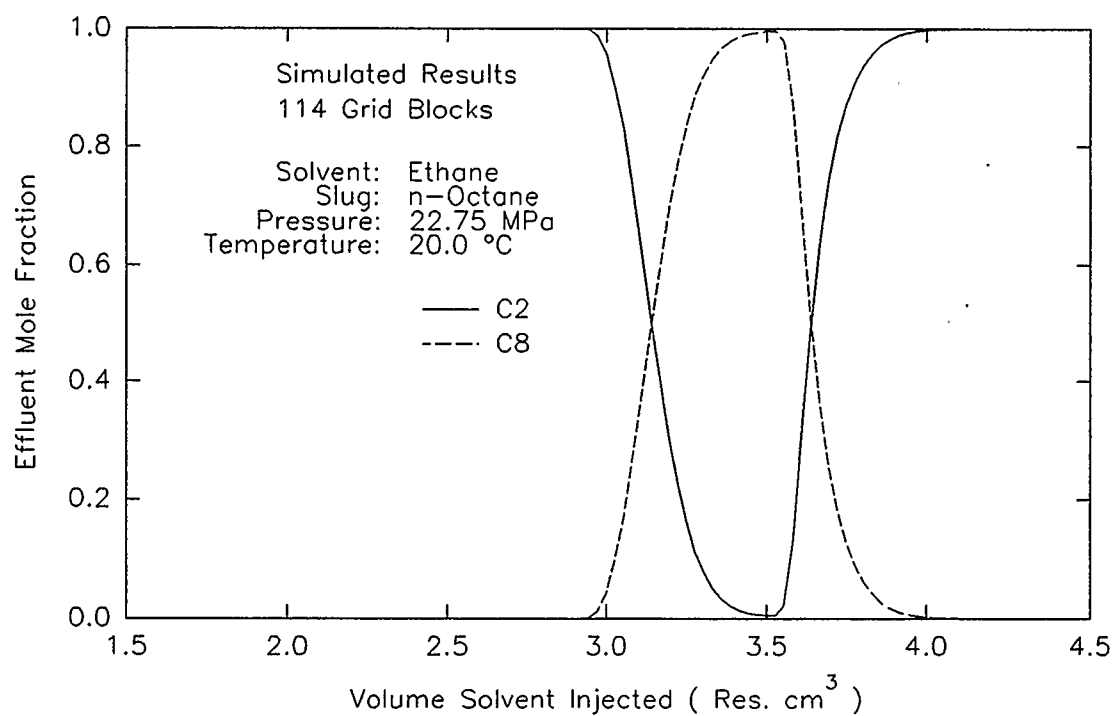


Figure 2.12: Taylor Dispersion Experiment - Ethane plus n-Octane, 20° C

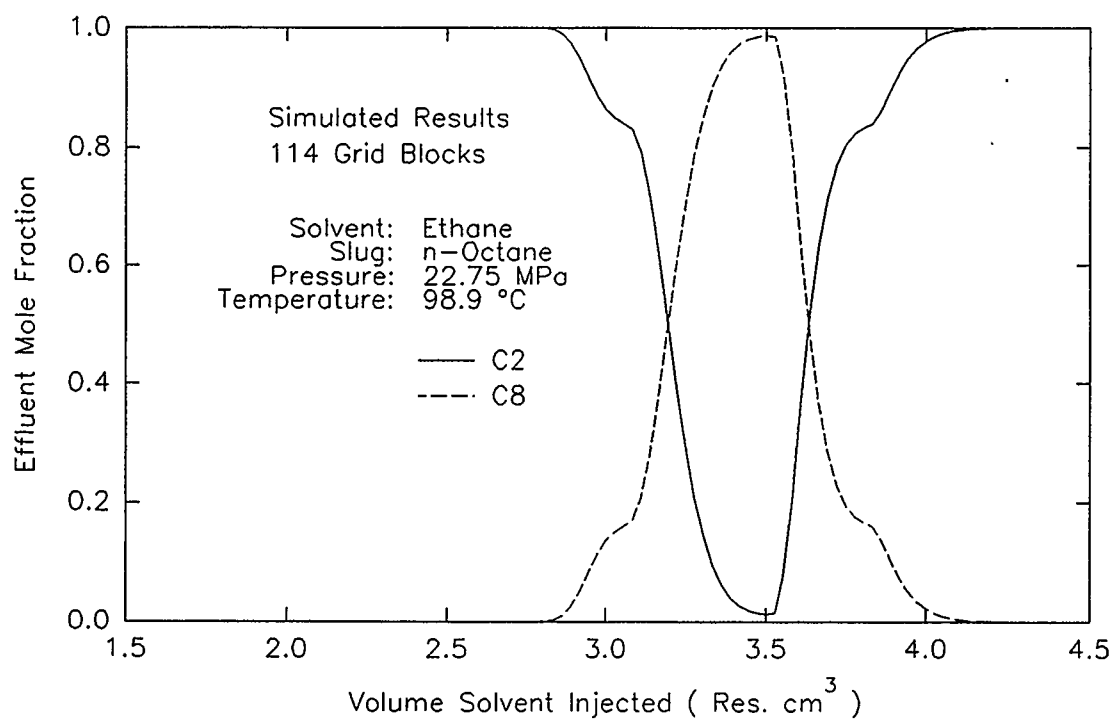


Figure 2.13: Taylor Dispersion Experiment - Ethane plus n-Octane, 100° C

3. RESERVOIR SIMULATION MODEL DEVELOPMENT

The development of a computer program for simulating miscible flooding operations in petroleum reservoirs is described in this Chapter. The formulation presented by Nghiem et al. (1981) is followed closely, although some minor modifications are made.

The program was developed in order to have a basic tool for reservoir simulation in which a variety of schemes for accounting for dispersion can be inserted. In addition to the ability to implement subroutines for dispersion calculations in the simulation model, it is also desirable to have control over the type of numerical dispersion control and automatic time step control schemes.

The model is developed by first deriving the differential equation for flow in porous media. The source/sink terms through dispersion is introduced are included in the mass balance equations. The discretization of the equations and the schemes for controlling numerical dispersion are described.

The assumptions employed in the model development and the approaches to calculating thermodynamic and transport properties are also dealt with.

3.1. MODEL EQUATIONS

3.1.1. FLOW EQUATIONS

3.1.1.1. Governing Differential Equation for Flow in Porous Media

As this model is to be used specifically for the simulation of hydrocarbon flooding processes, the mobility of water is not considered. Water saturation will be set to zero or to a constant value for all grid blocks equal to the irreducible water saturation. The flow equations are derived assuming two-phase multicomponent hydrocarbon flow. The

reservoir flow equations are derived from the continuity equation on a component basis. The equations express mass conservation, and symbols with a "tilde" ($\sim$) overmark should be understood to have mass units. These quantities will be converted to molar units for implementation in the simulator.

The continuity equation for a component m is given by Aziz and Settari (1979; p. 8) as:

$$-\nabla \cdot \dot{\mathbf{m}}_m = \frac{\partial \tilde{\rho}_m}{\partial t} - \tilde{q}_m \quad (3.1)$$

The mass flux may be written as the sum of the convective and dispersive fluxes:

$$\dot{\mathbf{m}}_m = x_m \tilde{\rho} \mathbf{u} + \mathbf{j}_m \quad (3.2)$$

where the first term on the right hand side above is the flux of component m associated with the bulk convective flux and the second term is the dispersive flux. The dispersive flux may be written in a form analogous to Fick's first law as follows (Young, 1984):

$$\mathbf{j}_m = -\mathbf{D}_m \nabla(\tilde{\rho} x_m) \quad (3.3)$$

where $\mathbf{D}_m$ is a dispersion tensor for component m . The elements of this dispersion tensor can contain contributions from both molecular diffusion and mechanical dispersion. Using equation (3.3), the mass flux for a two hydrocarbon phase system can be written as follows:

$$\mathbf{u}_m = x_{mo} \tilde{\rho}_o \mathbf{u}_o + x_{mg} \tilde{\rho}_g \mathbf{u}_g - \mathbf{D}_{mo} \nabla(\tilde{\rho}_o x_{mo}) - \mathbf{D}_{mg} \nabla(\tilde{\rho}_g x_{mg}) \quad (3.4)$$

The convective flow terms are calculated according to Darcy's law for the flow of fluids through porous media. This has been shown to be empirically equivalent to the Navier-Stokes equations and is valid for Newtonian fluids with a porous medium Reynolds number less than one and no inertial or slip effects occurring (Greenkorn, 1983; p.8). The

superficial, or Darcy, velocity of a phase j flowing simultaneously with one or more other phases is given as (Aziz and Settari, 1979; p. 12):

$$\mathbf{u}_j = \frac{-Kk_{rj}}{\mu_j} (\nabla P_j - \tilde{\rho}_j g \nabla z) \quad (3.5)$$

Applying this equation gives the final form of the mass flux term for two-phase hydrocarbon flow:

$$\begin{aligned} \dot{\mathbf{m}}_m = & -x_{mo} \tilde{\rho}_o \frac{Kk_{ro}}{\mu_o} (\nabla P_o - \tilde{\rho}_o g \nabla z) - x_{mg} \tilde{\rho}_g \frac{Kk_{rg}}{\mu_g} (\nabla P_g - \tilde{\rho}_g g \nabla z) \\ & - \mathbf{D}_{mo} \nabla(\tilde{\rho}_o x_{mo}) - \mathbf{D}_{mg} \nabla(\tilde{\rho}_g x_{mg}) \end{aligned} \quad (3.6)$$

The density term for two phases in a porous medium will be

$$\tilde{\rho}_m = \phi S_o \tilde{\rho}_o x_{mo} + \phi S_g \tilde{\rho}_g x_{mg} \quad (3.7)$$

and the capillary pressure relating the gas and oil pressures is given by:

$$P_{cog} = P_g - P_o \quad (3.8)$$

Inserting the flux and accumulation relationships into equation (3.1) gives the governing differential equation describing mass continuity of component m in the reservoir in terms of oil phase pressure, and flow and diffusion coefficients:

$$\begin{aligned} & \nabla \cdot \left[\frac{Kk_{ro} \tilde{\rho}_o x_{mo}}{\mu_o} (\nabla P_o - \tilde{\rho}_o g \nabla z) \right] + \nabla \cdot \left[\frac{Kk_{rg} \tilde{\rho}_g x_{mg}}{\mu_g} (\nabla P_g + \nabla P_{cog} - \tilde{\rho}_g g \nabla z) \right] \\ & + \nabla \cdot \mathbf{D}_{mo} \nabla(\tilde{\rho}_o x_{mo}) + \nabla \cdot \mathbf{D}_{mg} \nabla(\tilde{\rho}_g x_{mg}) \\ & = \frac{\partial}{\partial t} (\phi S_o \tilde{\rho}_o x_{mo} + \phi S_g \tilde{\rho}_g x_{mg}) - \tilde{q}_m \end{aligned} \quad (3.9)$$

To generalize this equation for use in one-, two- or three-dimensional problems, it must be multiplied by a geometric factor, α (Peaceman, 1977; p. 7):

$$\begin{aligned} \text{one dimension:} \quad & \alpha = A(x) \quad \text{reservoir cross-sectional area at } x \\ \text{two dimensions:} \quad & \alpha = H(x, y) \quad \text{reservoir vertical height at } x, y \\ \text{three dimensions:} \quad & \alpha = 1 \end{aligned} \quad (3.10)$$

As discussed in Chapter 2, conventional compositional simulators do not explicitly include dispersion. For this simulator, the normal development of the flow equation in which the diffusion terms are removed from equation (3.9) is followed at this point, allowing solution of the flow equation including only convective terms. Models for determining diffusive or dispersive flux separately from the convective flux are developed in Chapters 4 and 5. These dispersion terms will be added to the convection equation as sources or sinks for each grid block.

The final molar balance flow equation is derived from equation (3.9) by deleting the diffusion terms, multiplying through by the geometric factor given in equation (3.10) and dividing through by the molar mass of component m . The molar balance relating mole fractions in each phase to the global mole fraction is also used to allow simplification of the accumulation term. This gives the following result:

$$\begin{aligned} & \nabla \cdot \left[\frac{\alpha K k_{ro} \rho_o y_{mo}}{\mu_o} (\nabla P_o - \tilde{\rho}_o g \nabla z) \right] + \nabla \cdot \left[\frac{\alpha K k_{rg} \rho_g y_{mg}}{\mu_g} (\nabla P_o + \nabla P_{cog} - \tilde{\rho}_g g \nabla z) \right] \\ &= \alpha \frac{\partial}{\partial t} \left[\phi (\rho_o S_o + \rho_g S_g) z_m \right] - \alpha \hat{q}_m \end{aligned} \quad (3.11)$$

3.1.1.2. Discretized Form of Flow Equation

The flow equations are discretized to generate algebraic equations for each grid block. The derivatives in distance are evaluated using a backward difference discretization, and the derivatives in time are evaluated using a forward difference discretization. The differencing scheme and notation shown in the following equations is as given by Nghiem et al. (1981). The superscript n denotes the time level with time level n being the beginning of a time step, and time level $n+1$ being the end of a time step. The discretized mole balance for a hydrocarbon component m is given as:

$$\begin{aligned}
& \Delta \left[T_o^n y_{mo}^n (\Delta P_o^{n+1} - \tilde{\rho}_o^n g \Delta z) + T_g^n y_{mg}^n (\Delta P_o^{n+1} + \Delta P_{cog}^n - \tilde{\rho}_g^n g \Delta z) \right] + q_m \\
& = \frac{V_b}{\Delta t} \left[\phi^{n+1} (\rho_o S_o + \rho_g S_g)^{n+1} z_m^{n+1} - \phi^n (\rho_o S_o + \rho_g S_g)^n z_m^n \right]
\end{aligned} \tag{3.12}$$

The transmissibility terms, T , result from the coefficients multiplying the gradients in equation (3.11) and the discretization process, and are defined in section 3.3.4. The overall molar balance for the hydrocarbon system is obtained by summing equation (3.12) over all the hydrocarbon components:

$$\begin{aligned}
& \Delta \left[T_o^n (\Delta P_o^{n+1} - \tilde{\rho}_o^n g \Delta z) + T_g^n (\Delta P_o^{n+1} + \Delta P_{cog}^n - \tilde{\rho}_g^n g \Delta z) \right] + q_h \\
& = \frac{V_b}{\Delta t} \left[\phi^{n+1} (\rho_o S_o + \rho_g S_g)^{n+1} - \phi^n (\rho_o S_o + \rho_g S_g)^n \right]
\end{aligned} \tag{3.13}$$

The difference notation used in the above two equations is as follows:

$$\begin{aligned}
\Delta T \Delta P &= \Delta_x T_x \Delta P_x + \Delta_y T_y \Delta P_y + \Delta_z T_z \Delta P_z \\
\Delta_x T_x \Delta P_x &= T_{x,i+1/2} (P_{i+1} - P_i) - T_{x,i-1/2} (P_i - P_{i-1}) \\
\Delta t &= t^{n+1} - t^n
\end{aligned} \tag{3.14}$$

where the subscript i refers to grid block indices in the x direction. The differencing shown in equation (3.14) for the x direction is repeated for each geometric dimension in the simulation, and for each phase present in any given grid block. The evaluation of the transmissibilities, phase compositions, saturations and densities are detailed in the following sections of this chapter.

3.1.2. EQUILIBRIUM EQUATIONS

The gas and oil phases are assumed to be in equilibrium in all grid blocks. The thermodynamic equilibrium condition is expressed as the equality of component fugacities in the oil and gas phases:

$$f_{mo} = f_{mg}, \quad m = 1 \dots n_c \tag{3.15}$$

Further equations related to the equilibrium relation are derived from material balance on the hydrocarbon phases or result from the definition of mole fractions and saturations (volume fractions). The following equations are needed to complete the specification of the problem.

$$z_m = Ly_{mo} + Vy_{mg} \quad (3.16)$$

$$L = \frac{\rho_o S_o}{\rho_o S_o + \rho_g S_g} \quad (3.17)$$

$$V = \frac{\rho_g S_g}{\rho_o S_o + \rho_g S_g} \quad (3.18)$$

$$\sum_{m=1}^{n_c} z_m = \sum_{m=1}^{n_c} y_{mo} = \sum_{m=1}^{n_c} y_{mg} = 1 \quad (3.19)$$

$$L + V = 1 \quad (3.20)$$

$$S_o + S_g + S_w = 1 \quad (3.21)$$

3.2. SOLUTION OF MODEL EQUATIONS

3.2.1. OVERVIEW OF SOLUTION METHOD

Equation (3.13) is used to solve for the pressure in each grid block. At the beginning of the time step, a flash calculation is performed to obtain y_{mo} , y_{mg} , V , L , ρ_o and ρ_g . Transport properties for the calculation of the flow coefficients are also generated, and the well terms are evaluated. An approximate Jacobian is then constructed to allow the solution of the system of equations defined by (3.13). After the grid block pressures are calculated, equation (3.12) is solved for z_m , the flash calculation is repeated and the saturations are calculated from equations (3.17) or (3.18) and (3.21). The implicit terms in the pressure equation and the Jacobian are then updated and a new pressure vector is calculated until convergence is achieved.

3.2.2. FLASH CALCULATION

As the flash calculations for the hydrocarbon systems to be studied in this work are not expected to be difficult, a simple successive substitution algorithm will be used (e.g. Heidemann, 1983). The algorithm utilizes the acceleration procedure of Mehra et al. (1982) and the single- phase region determination procedure of Nghiem et al. (1983). The thermodynamic model used in the flash calculation is formulated as a general two-parameter cubic equation of state. Procedures for applying the Peng-Robinson (PR) equation (Peng and Robinson, 1976) and the Soave-Redlich-Kwong (SRK) equation (Soave, 1972) are given in the following section.

3.2.2.1. Equation of State

The general form of the cubic two-parameter equation of state is:

$$P = \frac{RT}{v - b} - \frac{a}{(v + c_1b)(v + c_2b)} \quad (3.22)$$

The gas constant R can be removed from the equation and from the formulas for the calculation of the pure component parameters by using the variable $v_R = v/R$. This approach has been used by Michelsen (1990) in phase behavior programs which were made available in the course of this work. The calculation of the equation of state constants and the constants in the pure component parameter formulas are due to Michelsen. The equation of state is now written as:

$$P = \frac{T}{v_R - b_R} - \frac{a_R}{(v_R + c_1b_R)(v_R + c_2b_R)} \quad (3.23)$$

The compressibility factor for a given phase

$$Z = \frac{Pv_R}{T} \quad (3.24)$$

is calculated as the solution of the equation of state expressed as cubic function of this variable:

$$Z^3 + [B(c_1 + c_2 - 1) - 1]Z^2 + [B^2(c_1c_2 - (c_1 + c_2)) - B(c_1 + c_2) + A]Z + (-B^3c_1c_2 - B^2c_1c_2 - AB) = 0 \quad (3.25)$$

The expression for determining the fugacity of a component m in a given phase is derived by substituting the pressure form of the equation of state into the following fundamental thermodynamic relationship:

$$RT \ln f_m = \int_V \left[\left(\frac{\partial P}{\partial n_m} \right)_{T,V,n \neq n_m} - \frac{RT}{V} \right] dV - RT \ln Z + RT \ln y_m P \quad (3.26)$$

The resulting component fugacity formula is:

$$\ln \frac{f_i}{y_i P} = \frac{b_i}{b} (Z - 1) - \ln(Z - B) + \frac{A}{B} \left[\frac{b_i}{b} - \frac{2 \sum_{j=1}^{n_c} y_j a_{ij}}{a} \right] \left(\frac{1}{c_1 - c_2} \right) \ln \left(\frac{Z + c_1 B}{Z + c_2 B} \right) \quad (3.27)$$

The pure component parameters for the above equations, following Michelsen's (1990) approach, are calculated as follows:

$$\begin{aligned} \alpha_i(T) &= 1 + m_i (1 - \sqrt{T/T_{ci}}) \\ a_i &= \Omega_a T_{ci} / P_{ci}^{1/2} \\ b_i &= \Omega_b T_{ci} / P_{ci} \\ a_{Ti} &= a_i \alpha_i(T) \\ a_{Ti,j} &= (1 - k_{ij}) a_{Ti} a_{Tj} \end{aligned} \quad (3.28)$$

and the mixture parameters are given by:

$$\begin{aligned}
a_R &= \sum_{i=1}^{n_c} \sum_{j=1}^{n_c} y_i y_j a_{Ti,j} \\
b_R &= \sum_{i=1}^{n_c} y_i b_i \\
A &= \frac{a_R P}{T^2} \\
B &= \frac{b_R P}{T}
\end{aligned} \tag{3.29}$$

The additional formulas required to use the SRK or PR equations are as follows. The relation used for the temperature dependence of the a parameter in the PR equation is the one in the original reference. For the SRK equation, the fit proposed by Graboski and Daubert (1978) is used:

$$\begin{aligned}
\text{SRK: } m_i &= 0.48508 + \omega_i(1.55171 - 0.15613\omega_i) \\
\text{PR: } m_i &= 0.37464 + \omega_i(1.54226 - 0.26992\omega_i)
\end{aligned} \tag{3.30}$$

The equation of state constants c_1 and c_2 are calculated according to

$$\begin{aligned}
\text{SRK: } c &= 0, \quad \text{PR: } c = 1 \\
u &= 1 + c \\
w &= -c \\
c_2 &= \frac{u + \sqrt{u^2 - 4w}}{2} \\
c_1 &= w/c_2
\end{aligned} \tag{3.31}$$

and finally the constants for the pure component a and b parameters are evaluated from:

$$\begin{aligned}
s_1 &= \frac{(u+w)(u+3)-w}{2} + 1 & s_2 &= u + w + 1 \\
q &= \left(s_1 + \sqrt{s_1^2 - s_2^3}\right)^{1/3} & r &= q + \frac{s_2}{q} + 1 \\
\Omega_b &= \frac{1}{3r + u - 1} & \Omega_a &= \Omega_b \sqrt{r(r^2 - 3w) - uw}
\end{aligned} \tag{3.32}$$

3.2.2.2. Flash Algorithm

The steps of the flash algorithm are outlined below. The initial data required are the pressure and temperature of the flash, feed composition, and critical pressure and temperature, acentric factors for each component and the binary interaction parameters.

1. Initial estimates of the K-factors are generated. At the beginning of a time step, the K-factors for each grid block are set to the final values obtained from the previous time step. Within the time step, the K-factors are set to the values obtained from the previous iteration of the pressure equation. At initialization of the program, the K-factors are estimated from the empirical relationship given by Wilson (1969):

$$K_i = \frac{\exp[5.37(1 + \omega_i)(1 - T_{ci}/T)]}{P/P_{ci}} \quad (3.33)$$

2. Vapor fraction is calculated. A mole balance on component i , coupled with the constraint that mole fractions within a phase must sum to one, yields a function in terms of the feed composition, K-factors and mole fraction vapor in the system:

$$f(V) = \sum_{i=1}^{n_c} \left[\frac{(K_i - 1)z_i}{1 + V(K_i - 1)} \right] = 0 \quad (3.34)$$

This equation is solved using Newton's method:

$$V^{(l+1)} = V^{(l)} - f(V^{(l)}) / f'(V^{(l)}) \quad (3.35)$$

where

$$f'(V) = - \sum_{i=1}^{n_c} \left[\frac{(K_i - 1)^2 z_i}{(1 + V(K_i - 1))^2} \right] \quad (3.36)$$

This approach will work as long as the K values are such that a solution for the vapor fraction lies between zero and one. If this is not the case, the function in (3.34) is used to

set the single-phase vapor or liquid fraction as follows (Nghiem et al., 1983): if $f(0) < 0$ then $V=0$, if $f(1) > 0$ then $V=1$; on the first iteration, the vapor fraction is set to $V=0.5$.

3. Component mole fractions in each phase are calculated.

$$\begin{aligned} y_{io} &= \frac{z_i}{1 + V(K_i - 1)}; \quad i = 1 \dots n_c \\ y_{ig} &= y_{io} K_i; \quad i = 1 \dots n_c \end{aligned} \quad (3.37)$$

These are normalized to ensure the mole fractions sum to one:

$$y_{io} = \frac{y_{io}}{\sum_{j=1}^{n_c} y_{jo}}, \quad y_{ig} = \frac{y_{ig}}{\sum_{j=1}^{n_c} y_{jg}}; \quad i = 1 \dots n_c \quad (3.38)$$

4. Fugacity of components in each phase are evaluated. First the equation of state parameters for each phase are calculated from equations (3.28) and (3.29). The cubic equation (3.25) is solved for each phase to generate the compressibility factors, then the fugacities of each component in both phases are calculated from equation (3.27).

5. Convergence check. The equilibrium criterion of equal component fugacities in both phases is checked according to:

$$\left[\sum_{i=1}^{n_c} \ln(f_{io}/f_{ig}) \right]^2 < 10^{-14} \quad (3.39)$$

If this criterion is met, the final step in the algorithm is the calculation of phase densities as follows:

$$\rho_j = \frac{Z_j}{PRT}; \quad j = o, g \quad (3.40)$$

If the convergence criterion is not met, the acceleration parameter (Mehra et al., 1982) is calculated as

$$\gamma^{(l)} = \left| \frac{\mathbf{g}^{(l-1)T} \mathbf{g}^{(l-1)}}{\mathbf{g}^{(l-1)T} (\mathbf{g}^{(l)} - \mathbf{g}^{(l-1)})} \right| \gamma^{(l-1)} \quad (3.41)$$

where

$$g_i = \ln f_{ig} - \ln f_{io} \quad (3.42)$$

The K-factors are then updated according to:

$$K_i^{(l+1)} = K_i^{(l)} \left[(f_{io}/f_{ig})^{(l)} \right]^{\gamma^{(l)}} \quad (3.43)$$

and the algorithm returns to step 2.

3.2.3. SATURATION CALCULATION

As discussed in 3.2.1, the water saturation will be set to zero or to a constant value equal to the irreducible water saturation. The saturations are calculated according to the constraint equations (3.17), (3.18) and (3.21). If the flash calculation yields a two-phase system, the oil saturation is calculated as:

$$S_o = \frac{(1 - S_w) L \rho_g}{L \rho_g + V \rho_o} \quad (3.44)$$

and the gas phase saturation is then

$$S_g = 1 - S_o - S_w \quad (3.45)$$

If a single phase system is encountered, then

$$S_g [\text{or } S_o] = 0 \quad (3.46)$$

leaving

$$S_o [\text{or } S_g] = 1 - S_w \quad (3.47)$$

3.2.4. FLOW COEFFICIENTS

The term flow coefficient refers to the transmissibility composition product seen in equation (3.12). The transmissibility is defined as:

$$T_j = \frac{A}{\Delta l} \frac{Kk_{rj}\rho_j}{\mu_j}, \quad j = o, g \quad (3.48)$$

where the area is that of the interface between two grid blocks with center to center distance given by Δl . The absolute permeability is calculated using a harmonic average of the two grid blocks. The other parameters in the transmissibility equation are evaluated using a single point upstream weighting method; that is, they are evaluated at the pressure and composition of the block with the higher pressure. The molar density of the phase is returned from the flash calculation. The relative permeability and viscosity calculations are described below

3.2.4.1. Viscosity Calculation

The viscosities of components with carbon number 6 or lower are calculated using the correlation of Jossi et al. (1962), derived from corresponding states and dimensional analysis. The viscosity of the C_6^- fraction is given by

$$\begin{aligned} \left[(\mu - \mu^*)\xi + 0.0001 \right]^{0.25} = & 0.1023 + 0.23364\rho_R \\ & + 0.058533\rho_R^2 - 0.40758\rho_R^3 + 0.0093324\rho_R^4 \end{aligned} \quad (3.49)$$

The parameters in this equation are calculated from:

$$\begin{aligned} \xi &= \frac{[\sum y_j T_{c,j}]^{1/6}}{[\sum y_j MW_j]^{1/2} [\sum y_j P_{c,j}]^{2/3}} \\ \rho_R &= \frac{\sum y_j v_{c,j}}{\sum y_j v_j} \end{aligned} \quad (3.50)$$

where T_c is in K and P_c is in atm. The low pressure gas mixture viscosity is calculated from

$$\mu^* = \frac{\sum y_j \mu_j^* MW_j}{\sum y_j MW_j} \quad (3.51)$$

and the individual component low pressure viscosity is given by

$$\begin{aligned} \mu_j^* \xi_j &= 3.4 \times 10^{-4} (T/T_{c,j})^{0.94} & (T/T_{c,j}) \leq 1.5 \\ \mu_j^* \xi_j &= 1.778 \times 10^{-4} [4.58(T/T_{c,j}) - 1.67]^{0.625} & (T/T_{c,j}) > 1.5 \end{aligned} \quad (3.52)$$

$$\xi_j = \frac{T_{c,j}^{1/6}}{MW_j^{1/2} P_{c,j}^{2/3}}$$

The viscosities of components or fractions characterized with carbon numbers of 7 or higher are calculated according to a correlation given by Shealy (1988), based on an empirical fit of pure component, distillation fraction, whole crude oil, and bitumen and tar data as a function of molecular weight. The individual component viscosities are corrected for the effect of temperature, combined to give the viscosity of the entire C_7^+ fraction, which is then corrected for the effect of pressure. Shealy also presents a mixing rule for combining the results of the C_6^- and the C_7^+ fractions.

3.2.4.2. Relative Permeability

As the water phase is either immobile or not present in the simulations, only two-phase relative permeabilities need be determined. A simple model for hydrocarbon phase relative permeabilities without oil or gas residual saturations is used as follows:

$$k_{rj} = \left[\frac{S_j}{1 - S_w} \right]^\beta, \quad j = o, g \quad (3.53)$$

This is similar to the approach used by Sigmund et al. (1979). As the oil and gas phases approach miscibility, the relative permeability curves approach straight lines, i.e. $\beta = 1$ (Nghiem et al.; 1981); under immiscible conditions, the relative permeability relation shows considerable curvature and a parameter of $\beta = 2$ may be used.

3.2.5. NUMERICAL DISPERSION CONTROL

Depending on the model chosen for implementing physical dispersion, some mechanism for controlling numerical dispersion may be required. Evaluating the compositions which multiply the transmissibilities in equation (3.12) at the upstream grid block will be referred to as operating without numerical dispersion control. The scheme proposed by Nghiem et al. (1981) to control numerical dispersion, i.e., a two-point upstream weighting scheme for these compositions, will be used here. If $i-1$ and $i-2$ are the two upstream grid blocks from block i , the desired composition at the interface $i-1/2$ is obtained by extrapolating the compositions in the two upstream blocks to that interface, using the relation

$$y_{m,i-1/2} = y_{m,i-1} + \frac{\Delta I_{i-1}}{\Delta I_{i-1} + \Delta I_{i-2}} (y_{m,i-1} - y_{m,i-2}) \quad (3.54)$$

subject to the following constraints:

$$y_{m,i-1/2} \leq \max(y_{m,i-1}, y_{m,i}) \quad (3.55)$$

and

$$y_{m,i-1/2} \geq \min(y_{m,i-1}, y_{m,i}) \quad (3.56)$$

These equations will apply to both the oil and gas phases in a grid block. If only one phase is present, the global composition will be used.

3.2.6. SOURCE AND SINK TERMS

In a conventional compositional reservoir simulator, the only source and sink terms are the injection and production wells. For the applications considered here, dispersion or diffusion may be evaluated explicitly and added to the flow equation. The source/sink term in equation (3.12) will be the sum of the net dispersive molar flow rate and the molar flow rate resulting from injection or production wells.

$$q_m = q_{d,m} + q_{w,m} \quad (3.57)$$

Evaluation of the dispersive term will be discussed in Chapter 5.

The molar flow rate of hydrocarbon component m flowing into or out of a grid block i will be given by:

$$q_{w,m} = y_{mo}^n \rho_o^n Q_o^n + y_{mg}^n \rho_g^n Q_g^n \quad (3.58)$$

The rates are positive for injection wells (flow into the grid block) and negative for production wells by convention. For constant rate injection wells, the volumetric flow rate and composition of the injected fluid are specified. The density of the fluid is evaluated at the oil pressure of the grid block. For constant-rate production wells, the volumetric flow rate is specified and the composition and density are those of the i th grid block.

For constant bottomhole pressure wells, the volumetric flow rates are given by:

$$Q_j = I_{wj} (P_{bh} - P_{o,i}^{n+1}) \quad (3.59)$$

with the well index calculated from (Aziz and Settari; 1979, p. 223):

$$I_{wj} = \frac{2\pi\lambda\Delta z}{\ln(r_{eq}/r_w) - c} \quad (3.60)$$

where the mobility of a phase j is defined as

$$\lambda_j = \frac{k_{rj}}{\mu_j} \quad (3.61)$$

and the total mobility of fluids in a grid block is defined as the sum of the mobilities of each phase present. For injection wells or sources, the mobility term in equation (3.60) will be the total mobility of fluids in the grid block. For production wells or sinks, the mobility will be that of the phase j in the grid block.

3.2.7. PRESSURE EQUATION SOLUTION

The vector of grid block pressures is solved for by writing equation (3.13) for each grid block in the following form:

$$F_i = \Delta \left[T_o^n (\Delta P_o^{n+1} - \tilde{\rho}_o^n g \Delta z) + T_g^n (\Delta P_o^{n+1} + \Delta P_{\text{cog}}^n - \tilde{\rho}_g^n g \Delta z) \right] + q_h - \frac{V_b}{\Delta t} \left[\phi^{n+1} (\rho_o S_o + \rho_g S_g)^{n+1} - \phi^n (\rho_o S_o + \rho_g S_g)^n \right] = 0 \quad (3.62)$$

The solution of the grid block pressures at time level $n+1$ is accomplished using a Newton-type iteration with an approximate Jacobian. Given the l th iterate of $P_{o,i}^{n+1}$ ($P_{o,i}^{(l)}$), the $(l+1)$ th iterate is obtained from:

$$\sum_k J_{ik}^{(l)} [P_{o,k}^{(l+1)} - P_{o,k}^{(l)}] = -F_i^{(l)}, \quad i = 1 \dots n_b \quad (3.63)$$

The sum is taken over the i th grid block and all adjacent blocks. The elements of the Jacobian are given by:

$$J_{ik}^{(l)} = \left(\frac{\partial F_i}{\partial P_{o,k}} \right)^{(l)} = (T_o + T_g)_{(i+k)/2}^n \quad (3.64)$$

and

$$J_{ii}^{(l)} = \left(\frac{\partial F_i}{\partial P_{o,i}} \right)^{(l)} = - \sum_{\substack{k \\ k \neq i}} (T_o + T_g)_{(i+k)/2}^n + \left(\frac{\partial q_h}{\partial P_o} \right)_i^{(l)} - \frac{V_{b,i}}{\Delta t} \left[\frac{\partial \phi (\rho_o S_o + \rho_g S_g)}{\partial P_o} \right]_i^{(l)} \quad (3.65)$$

The derivatives of the source and sink terms are derived from equations (3.57) through (3.60). As these derivatives are taken with respect to the l th iterate of the pressure at time level $(n+1)$, terms which are evaluated explicitly will have zero derivatives. Thus for rate constrained wells

$$\frac{\partial q_h}{\partial P_o^{n+1}} = 0 \quad (3.66)$$

while for pressure constrained wells

$$\frac{\partial q_h}{\partial P_o^{n+1}} = -I_{wo}\rho_o - I_{wg}\rho_g \quad (3.67)$$

The derivatives of the accumulation term in equation (3.68) are evaluated following the method of Nghiem et al. (1981), with the additional assumption of constant porosity. As the densities are functions of pressure and composition, true derivatives of the accumulation term will involve derivatives of composition with respect to pressure as well as derivatives of saturation with respect to pressure. An approximation to the derivative of the accumulation term is obtained by neglecting these terms, leaving the following:

$$\left[\frac{\partial \phi(\rho_o S_o + \rho_g S_g)}{\partial P_o} \right]_i^{(l)} \cong \phi \left(S_o \frac{\partial \rho_o}{\partial P_o} + S_g \frac{\partial \rho_g}{\partial P_o} \right)_i^{(l)} \quad (3.68)$$

The derivatives of density with respect to pressure are evaluated using

$$\frac{\partial \rho_j}{\partial P_o} = \left[-v_j^2 \frac{\partial P_o}{\partial v_j} \right]^{-1} \quad (3.69)$$

where the derivative of pressure with respect to volume is obtained from the form of the equation of state given in equation (3.23):

$$\frac{\partial P_o}{\partial v} = \frac{1}{R} \frac{\partial P_o}{\partial v_R} = \frac{-T}{R(v_R - b)^2} + \frac{a(2v_R + (c_1 + c_2)b)}{R((v_R + c_1b)(v_R + c_2b))^2} \quad (3.70)$$

This construction yields an approximate Jacobian which is symmetric and diagonally dominant. As only oil pressure is being solved for implicitly, capillary pressure and gravitational effects being taken into account explicitly, this formulation results in simple tri-diagonal matrices for one-dimensional problems and penta-diagonal matrices for two-dimensional problems. These are easily solved using direct elimination methods.

3.2.8. COMPOSITION EQUATION SOLUTION

Once the $(l+1)$ th iterate of the pressure vector is evaluated, the composition corresponding to this pressure is evaluated. Defining:

$$\Delta \Phi_o^{(l+1)} = \Delta P_o^{(l+1)} - \tilde{\rho}_o^n g \Delta z \quad (3.71)$$

and

$$\Delta \Phi_g^{(l+1)} = \Delta P_o^{(l+1)} + \Delta P_{cog}^n - \tilde{\rho}_g^n g \Delta z \quad (3.72)$$

the composition equation is obtained by rearranging equation (3.12) to give:

$$z_m^{(l+1)} = \frac{\left\{ \Delta \left[T_o^n y_{mo}^n \Delta \Phi_o^{(l+1)} + T_g^n y_{mg}^n \Delta \Phi_g^{(l+1)} \right] + q_m + \frac{V_b}{\Delta t} \phi(\rho_o S_o + \rho_g S_g)^n z_m^n \right\}}{\frac{V_b}{\Delta t} \phi(\rho_o S_o + \rho_g S_g)^{(l+1)}} \quad (3.73)$$

The term in the denominator is evaluated from equation (3.13):

$$\frac{V_b}{\Delta t} \phi^{(l+1)}(\rho_o S_o + \rho_g S_g)^{(l+1)} = \Delta \left[T_o^n \Delta \Phi_o^{(l+1)} + T_g^n \Delta \Phi_g^{(l+1)} \right] + q_h + \frac{V_b}{\Delta t} \phi(\rho_o S_o + \rho_g S_g)^n \quad (3.74)$$

Calculating the composition in this way guarantees that the mole fractions will sum to unity.

3.2.9. AUTOMATIC TIME STEP SIZE CONTROL

In addition to the use of upstream weighting techniques for numerical dispersion control, IMPES techniques may benefit from the use of maximal time steps, provided they are less than the size required to satisfy the throughput stability criterion. Aziz and Settari (1979; p. 156) show that for single point upstream weighting, use of a time step exactly equal to the stability limit can eliminate the first order term in the truncation error; they go on to state that " In general, truncation errors with upstream explicit transmissibility will be minimized by the use of the maximum stable time step". For the two-point upstream weighting technique, the coefficient of the first order time step size term is negative,

indicating that increasing the time step size will decrease the numerical dispersion. In this simulator several methods of automatic time step size control have been implemented.

Solution of the flow equations for the first time step is usually easiest with a small time step. A user-supplied initial time step is employed here. The other user supplied values are minimum and maximum allowable time step sizes, and maximum changes in mole fraction and pressure allowable for a grid block. The maximum allowable changes are useful for ensuring that transient conditions that the user wishes to see are not obscured by the simulator taking time steps that are too large. A typical value for maximum allowable mole fraction change in a compositional simulator is 0.2, while the maximum pressure change will depend on the absolute pressures expected in the simulation.

At the end of a time step, the maximum changes in pressure and composition are compared to the allowable limits. If any change exceeds the allowables, the time step size is multiplied by $2/3$ for the next step. If the maximum changes are both less than 50% of the allowables, the time step size is multiplied by 1.5. These operations are carried out only within the limits set by the user for minimum and maximum time step sizes.

As potentially large amounts of material may be transferred across a grid block interface through dispersion when the model is applied to enhanced dispersion problems, the net removal of moles of a component expected for a grid block over a time step is checked at the beginning of the step to ensure it will not be more than the number of moles initially contained in the grid block. As the dispersive rates are set explicitly, the exact number of moles of material to be transferred through dispersion can be calculated. An estimate of the moles of a component to be transferred via convection can be obtained using the explicit transmissibilities and the values of pressure and density existing at the

beginning of the time step. If a grid block is determined to have a negative mole fraction of a component by this calculation, the time step size will be multiplied by 2/3.

3.3. SUMMARY

This Chapter has presented the details of a basic IMPES type compositional simulator. The simulator was set up in the usual manner and therefore does not include dispersion explicitly in the model equations. Physical dispersion has been added as source/sink terms in the equations. Numerical dispersion was controlled by two-point upstream weighting applied to the interface compositions.

The simulation program was used to produce the results described in Chapter 6 of this dissertation.

4. EVALUATION OF DIFFUSIVE FLUX

The use of Fick's laws of diffusion to evaluate the diffusive flux for reservoir simulation is discussed in this Chapter. Fick's first law is introduced as the basis of the mathematical treatment of diffusion. Green's function theory is used to develop a consistent methodology for the solution of the diffusion equation under various initial and boundary conditions. The application of prescribed flux boundary conditions results in a semi-analytical formulation for the concentration profile which may be solved either in the time or the Laplace domain. Although they are not used in the dispersive flux models in the reservoir simulator, the prescribed flux boundary condition solutions are introduced here since the source functions derived for these conditions are used in the infinite media or impermeable boundary solutions as well. For solutions of the diffusion equation which depend only on the initial conditions, that is where end effects are not important or where impermeable boundaries exist, analytical forms for the concentration profiles are developed. This allows closed forms for the derivatives and integrals of the profiles to be derived as well. In this Chapter, the solutions of the diffusion equation are derived which are the tools used in Chapter 5 for formulating the dispersive flux models for the reservoir simulator.

4.1. FICK'S LAWS OF DIFFUSION

The mathematical theory of diffusion in isotropic substances is described by two equations adapted by Fick from the equations of heat conduction (Crank, 1975). Fick's first law states that the rate of transfer of a diffusing substance is proportional to the concentration gradient measured normal to the direction of flow, while the second law is a continuity equation derived from the first law. The solution of these equations to give the diffusive flux for use in reservoir simulation is examined in this section.

4.1.1. FICK'S FIRST LAW

Fick's first law for a binary system of A and B , with a binary mass diffusion coefficient $D_{AB} = D_{BA}$, can be written to give the molar diffusive flux (Bird et al., 1960; p. 502) as follows:

$$j_A = -\rho D_{AB} \nabla y_A \quad (4.1)$$

For diffusion in a system of more than two components, the diffusive flux of a component i can be given in terms of multicomponent diffusion coefficients:

$$j_i = -\rho \sum_{k=1}^{n_c} D_{ik}^M \nabla y_k \quad (4.2)$$

The use of effective diffusion coefficients allows determination of the flux of one constituent of a multicomponent system while retaining the simplicity of the relationship for a binary system:

$$\mathbf{j}_i = -\rho D_i \nabla y_i \quad (4.3)$$

Evaluation of diffusive flux with this equation becomes simply a problem of determining the concentration gradient with distance at any point and applying equation (4.3).

4.1.2. FICK'S SECOND LAW: THE DIFFUSION EQUATION

The diffusion equation for one component in a multicomponent system can be obtained by writing the continuity relationship for component i , with the only driving force for component motion being the diffusive flux given by equation (4.3):

$$\frac{\partial \rho_i}{\partial t} = \nabla \cdot \rho D_i \nabla y_i \quad (4.4)$$

For constant diffusivity and density, this equation reduces to

$$\frac{\partial \rho_i}{\partial t} = D_i \nabla^2 \rho_i \quad (4.5)$$

The solution of this equation is uniquely determined when the initial concentration distribution and either a constant value of concentration on the boundary (Dirichlet problem), or prescribed flux across the boundary (Neumann problem) is defined. Green's function theory is introduced in the next section as a means to systematically develop solutions for various initial and boundary conditions.

4.2. THE USE OF GREEN'S FUNCTIONS FOR SOLUTION OF THE DIFFUSION EQUATION

4.2.1. OUTLINE OF GREEN'S FUNCTION THEORY

Green's function theory provides a methodology for solving linear differential equations with boundary conditions which consist of linear combinations of the unknowns and their derivatives. The procedure for solving ordinary differential equations is shown here. The procedure for partial differential equations is essentially the same, with the dimensionality of the integrals extended for additional variables.

The method is applicable for any general differential equation of the form:

$$\mathbf{L}u = \phi \quad (4.6)$$

over the interval $a \leq x \leq b$, where $\mathbf{L}$ is an n th order linear ordinary differential operator. The Green's function G , as yet undefined, is introduced by forming the inner product: $G\mathbf{L}u$. This quantity is then subjected to repeated integration by parts, in terms of a dummy integration variable ξ , until the result can be expressed in the form:

$$\int_a^b G\mathbf{L}u d\xi = [\dots]_a^b + \int_a^b u\mathbf{L}^*G d\xi \quad (4.7)$$

where $\mathbf{L}^*$ is the formal adjoint differential operator associated with $\mathbf{L}$. A boundary value problem on G is defined by setting.

$$\mathbf{L}^*G = \delta(\xi - x) \quad (4.8)$$

where $\delta(\xi - x)$ is the delta function acting with unit strength at the point $x = \xi$. This function has the property:

$$\int_{-\infty}^{\infty} \delta(\xi - x) h(\xi) d\xi = h(x) \quad (4.9)$$

where $h(x)$ is any smooth function. As a result of this property, the last term of equation (4.7) reduces to $u(x)$ when the definition of equation (4.8) is invoked. Thus, substituting (4.8) into the last term of (4.7), and recalling the definition of equation (4.6), gives the result:

$$\int_a^b G \phi d\xi = [\dots]_a^b + u(x) \quad (4.10)$$

Specification of the boundary value problem on G is completed by requiring that G satisfy homogeneous boundary conditions such that unspecified boundary values of u and its derivatives are eliminated from the boundary term in equation (4.10). The Green's function G is then found by solving equation (4.8) with these homogeneous boundary conditions. Once G is known, the solution of the original differential equation is found by evaluating the integral in equation (4.10).

4.2.2. APPLICATION OF GREEN'S FUNCTION METHOD TO THE DIFFUSION EQUATION

Rigorous derivation of the treatment of the diffusivity problem with Green's functions is available from a number of sources, e.g. Gringarten and Ramey (1973) and Greenberg (1971). In this section, one possible formulation of the integral equation is given.

The differential equation (4.5) giving the molar concentration of a component i as a function of that component's diffusivity is identical to the heat conduction equation giving the temperature of a substance as a function of its thermal diffusivity. The formulation of the Green's function solution for this problem is taken from Carslaw and Jaeger (1959; p. 353).

The Green's function will be the molar concentration of a component i at a location $\mathbf{x}$ and time t due to an instantaneous source of unit molar density of component i generated at $\mathbf{x}'$ and time τ . This solution may be written

$$G = f(\mathbf{x}, \mathbf{x}', t - \tau) \quad t > \tau \quad (4.11)$$

From equation (4.5), the linear differential operator form of the diffusion equation is:

$$\mathbf{L}\rho_i = \left[D_i \nabla^2 - \frac{\partial}{\partial t} \right] \rho_i = 0 \quad t > 0 \quad (4.12)$$

The resulting form of the equation in G with the adjoint differential operator is

$$\mathbf{L}^*G = \left[D_i \nabla^2 + \frac{\partial}{\partial \tau} \right] G = 0 \quad \tau < t \quad (4.13)$$

Since t appears in G only in the form $(t - \tau)$, G will also satisfy

$$\frac{\partial G}{\partial t} = D_i \nabla^2 G \quad t > \tau \quad (4.14)$$

thus, the Green's functions may be found as simple solutions of the diffusion equation.

Casting the differential equation for diffusion into integral form via the integration by parts procedure outlined above results in the following solution:

$$\begin{aligned} \rho_i(\mathbf{x}, t) = & \iiint \rho_i(\mathbf{x}', t = 0) G(\mathbf{x}, \mathbf{x}', t) d\mathbf{x}' \\ & + D_i \int_0^t \left[\iiint \left(G(\mathbf{x}, \mathbf{x}', t - \tau) \frac{\partial \rho_i(\mathbf{x}', \tau)}{\partial \mathbf{n}} - \rho_i(\mathbf{x}', \tau) \frac{\partial G(\mathbf{x}, \mathbf{x}', t - \tau)}{\partial \mathbf{n}} \right) d\mathbf{x}' \right] d\tau \end{aligned} \quad (4.15)$$

where the derivatives with respect to $\mathbf{n}$ indicate differentiation normal to the boundary. The first integral above reflects the response due to the initial concentration distribution, and is taken over the entire domain of the problem. The second integral may reflect the response to either a prescribed concentration on the boundary or a prescribed flux across the boundary of the problem domain, and is taken over the surface of the domain only. For a prescribed concentration boundary condition, the Green's function vanishes on the boundary; this is a Green's function of the first kind. For the prescribed flux boundary condition the Green's function normal derivative will be zero on the boundary, giving a Green's function of the second kind. Equation (4.15) thus provides a "master equation" which may be simplified systematically for the solution of the diffusion equation under various conditions. Once the boundary and initial conditions for a problem are set, the Green's function is found as the solution of equation (4.14), this is then substituted into the appropriate simplified form of equation (4.15), to obtain the solution for the concentration distribution at any time. Solutions for flux boundary conditions and some general initial conditions are given in the following sections.

4.3. SOLUTIONS OF THE DIFFUSION EQUATION WITH PRESCRIBED FLUX BOUNDARY CONDITIONS

4.3.1. INTEGRAL EQUATION FORMULATION

The solution of the general integral equation (4.15) can be written in terms of a variation in concentration from the initial condition as follows:

$$\Delta\rho_i(\mathbf{x},t) = \rho_i(\mathbf{x},t) - \iiint \rho_i(\mathbf{x}',t=0)G(\mathbf{x},\mathbf{x}',t)d\mathbf{x}' \quad (4.16)$$

As described above, for flux boundary conditions the Green's function normal derivative is defined as being zero on the boundary of the domain, thus the second term in the boundary integral in equation (4.15) vanishes. Letting $N_j(\mathbf{x}',t)$ represent a general function

for the molar flux (moles/area-time) across the boundary, the normal derivative of the concentration can be expressed as

$$\frac{\partial \rho_i(\mathbf{x}', t)}{\partial \mathbf{n}} = \frac{N_i(\mathbf{x}', t)}{D_i} \quad (4.17)$$

and the integral equation can now be written

$$\Delta \rho_i(\mathbf{x}, t) = \int_0^t \left[\iint G(\mathbf{x}, \mathbf{x}', t - \tau) N_i(\mathbf{x}', \tau) d\mathbf{x}' \right] d\tau \quad (4.18)$$

This is the boundary integral formulation of the diffusion equation. A convolution integral in time of this form has also been derived by van Everdingen and Hurst (1949) for the pressure diffusion equation, relating transient pressure behavior in reservoirs to volumetric fluid offtake.

In general, numerical integration must be used for all but a few idealized flux functions in the solution of equation (4.18). Following van Kruijsdijk (1988), the Laplace transform of this equation may be taken to yield a considerably simplified form:

$$\Delta \bar{\rho}_i(\mathbf{x}, s) = \iint \bar{G}(\mathbf{x}, \mathbf{x}', s) \bar{N}_i(\mathbf{x}', s) d\mathbf{x}' \quad (4.19)$$

While eliminating the integral in time, use of this formulation does pose the problem of Laplace inversion. The source functions for use with equations (4.18) or (4.19) are derived in the following sections, and application of these source functions in the integral equations for one and two dimensional problems are discussed.

4.3.2. SOLUTION OF THE CONCENTRATION DIFFUSION EQUATION IN ONE DIMENSION

The diffusion equation will be solved for a one dimensional domain of length x_e and a constant cross-sectional area. The molar flux of component i (moles/area-time) across each end of the domain will be given as a general function of time, $f(t)$ at $x = 0$ and

$g(t)$ at $x = x_e$. For all of the problems with the flux boundary conditions, the initial condition is assumed to be a constant and uniform distribution of component i throughout the domain.

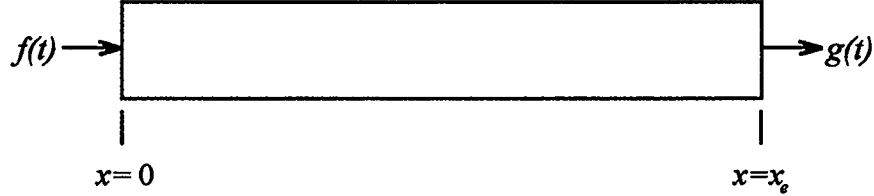


Figure 4.1: One Dimensional Problem Geometry

As discussed above, the integral equation will be used to give the result of the concentration distribution in terms of a variation from the initial condition. Specifying the initial condition as

$$\rho_i(x, t = 0) = \rho_i^o \quad 0 \leq x \leq x_e \quad (4.20)$$

equation (4.16) becomes

$$\Delta \rho_i(x, t) = \rho_i(x, t) - \rho_i^o \quad (4.21)$$

and the time domain diffusion equation from (4.5) may be written in one dimension directly for the change in concentration given in equation (4.21) as

$$\frac{\partial \Delta \rho_i(x, t)}{\partial t} = D_i \frac{\partial^2 \Delta \rho_i(x, t)}{\partial x^2} \quad t > 0 \quad (4.22)$$

The prescribed flux boundary conditions are

$$\begin{aligned} \left[\frac{\partial \Delta \rho_i(x, t)}{\partial x} \right]_{x=0} &= \frac{f(t)}{D_i} \quad t > 0 \\ \left[\frac{\partial \Delta \rho_i(x, t)}{\partial x} \right]_{x=x_e} &= \frac{g(t)}{D_i} \quad t > 0 \end{aligned} \quad (4.23)$$

and the initial condition for the transformed equation may now be given as

$$\Delta \rho_i(x, t = 0) = 0 \quad 0 \leq x \leq x_e \quad (4.24)$$

This transformation allows a consistent statement of the Laplace domain problem given below, where the zero initial condition is taken into account in the Laplace transformation of the differential equation.

$$D_i \frac{\partial^2 \Delta \bar{\rho}_i(x, s)}{\partial x^2} = s \Delta \bar{\rho}_i(x, s) \quad (4.25)$$

$$\begin{aligned} \left[\frac{\partial \Delta \bar{\rho}_i(x, s)}{\partial x} \right]_{x=0} &= \frac{\bar{f}(s)}{D_i} \\ \left[\frac{\partial \Delta \bar{\rho}_i(x, s)}{\partial x} \right]_{x=x_i} &= \frac{\bar{g}(s)}{D_i} \end{aligned} \quad (4.26)$$

4.3.3. TIME DOMAIN SOLUTION

4.3.3.1. Infinite Media Source Function

From equation (4.14), the differential equation to be solved for the source function is given by

$$\frac{\partial G(x, t)}{\partial t} = D_i \frac{\partial^2 G(x, t)}{\partial x^2} \quad t > \tau \quad (4.27)$$

Carslaw and Jaeger (1959; p. 259) present a solution based on Kelvin's treatment of instantaneous point sources. The response in an infinite linear region to an instantaneous plane source of strength unity acting at $t = 0$ and passing through x' , parallel to the plane at $x = 0$, will be given by:

$$G(x, x', t) = \frac{\exp\left[-(x - x')^2 / 4D_i t\right]}{2\sqrt{\pi D_i t}} \quad (4.28)$$

Gringarten (1971) derives the same relation by solving equation (4.27) using Laplace transformation with the following initial condition:

$$G(x, t = 0) = 0 \quad (4.29)$$

and boundary conditions:

$$\begin{aligned} G(x, t)|_{x=\infty} &= 0 \\ \left. \frac{\partial G(x, t)}{\partial x} \right|_{x=0} &= -\frac{1}{D_i} \end{aligned} \quad (4.30)$$

where the second boundary condition represents a unit molar flux sink at the origin.

4.3.3.2. Bounded Media Source Function

The source function for a bounded one dimensional domain can be derived from the infinite medium source function using the method of images. The region is assumed to have no-flow boundaries at $x = 0$ and $x = x_e$; for the purpose of creating the image system, the medium is assumed to be infinite. By the process of taking images in the bounding planes, a distribution of sources which gives a flux condition vanishing on the boundaries yet retaining the required sources within the domain is obtained. For the region with a source located at x' , the boundary at $x = 0$ is obtained by taking the image at $-x'$, that is, a source is placed at $-x'$ to counter the source at x' . To generate the boundary at $x = x_e$, the images of the sources at x' and $-x'$ must be considered with respect to this boundary. These in turn require two images with respect to the boundary at $x = 0$, and an infinite number of coupled plane sources results. A schematic diagram of this system of images is shown below in Figure 4.2.

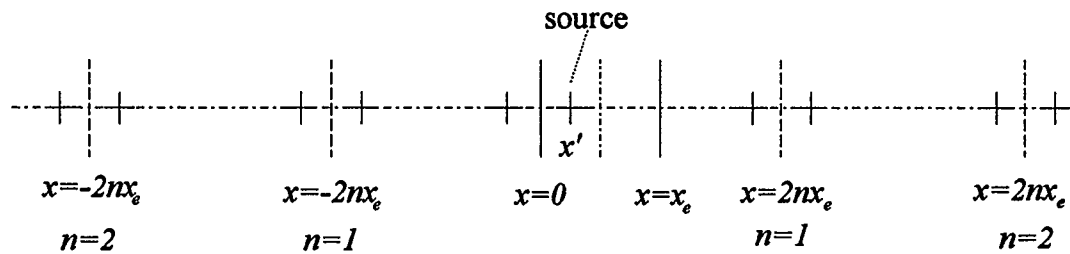


Figure 4.2: The Method of Images

The instantaneous source function for the system of sources shown above is equal to the sum of instantaneous source functions for each plane source. The image series equation resulting from this summation will be:

$$\begin{aligned}
 G(x, x', t) = & \frac{1}{2\sqrt{\pi D_i t}} \left\{ \exp\left[-(x - x')^2 / 4D_i t\right] + \exp\left[-(x + x')^2 / 4D_i t\right] \right\} \\
 & + \sum_{n=1}^{\infty} \frac{1}{2\sqrt{\pi D_i t}} \left\{ \exp\left[-(x - x' - 2nx_e)^2 / 4D_i t\right] + \exp\left[-(x + x' - 2nx_e)^2 / 4D_i t\right] \right\} \\
 & + \sum_{n=1}^{\infty} \frac{1}{2\sqrt{\pi D_i t}} \left\{ \exp\left[-(x - x' + 2nx_e)^2 / 4D_i t\right] + \exp\left[-(x + x' + 2nx_e)^2 / 4D_i t\right] \right\}
 \end{aligned} \quad (4.31)$$

This may be rearranged to give the following

$$\begin{aligned}
 G(x, x', t) = & \frac{1}{2\sqrt{\pi D_i t}} \sum_{n=-\infty}^{\infty} \left\{ \exp\left[-(x - x' + 2nx_e)^2 / 4D_i t\right] \right. \\
 & \left. + \exp\left[-(x + x' + 2nx_e)^2 / 4D_i t\right] \right\}
 \end{aligned} \quad (4.32)$$

Gringarten and Ramey (1973) present a number of source functions obtained in this way for different geometries and boundary conditions. They use Poisson's summation formula (Carslaw and Jaeger, 1959; p. 275):

$$\sum_{n=-\infty}^{\infty} \exp\left[-(x + 2na)^2 / 4\kappa t\right] = \frac{\sqrt{\pi\kappa t}}{a} \left\{ 1 + 2 \sum_{n=1}^{\infty} \cos \frac{n\pi x}{a} \exp\left[-\kappa n^2 \pi^2 t / a^2\right] \right\} \quad (4.33)$$

to transform equation (4.32), giving the source function for the finite one-dimensional domain with no-flow boundaries at $x = 0$ and $x = x_e$ and a source at point x' as follows:

$$G(x, x', t) = \frac{1}{x_e} \left[1 + 2 \sum_{n=1}^{\infty} \exp\left(\frac{-n^2 \pi^2 D_i t}{x_e^2}\right) \cos\left(\frac{n\pi x'}{x_e}\right) \cos\left(\frac{n\pi x}{x_e}\right) \right] \quad (4.34)$$

4.3.3.3. Application of the Integral Equation

To use equation (4.34) for the one-dimensional grid block with sources at each end, the boundary integral in equation (4.18) over the source domain becomes simply the

summation of two terms: one with the source function positioned at $x' = 0$, and the other with the source function positioned at $x' = x_e$. The final equation for generation of the one-dimensional concentration gradient is then given by

$$\Delta\rho_i(x,t) = \int_0^t [f(\tau)G(x,x' = 0,t - \tau) + g(\tau)G(x,x' = x_e,t - \tau)]d\tau \quad (4.35)$$

with the source functions defined by:

$$G(x,x' = 0,t) = \frac{1}{x_e} \left[1 + 2 \sum_{n=1}^{\infty} \exp\left(\frac{-n^2 \pi^2 D_i t}{x_e^2}\right) \cos\left(\frac{n\pi x}{x_e}\right) \right] \quad (4.36)$$

and

$$G(x,x' = x_e,t) = \frac{1}{x_e} \left[1 + 2 \sum_{n=1}^{\infty} \exp\left(\frac{-n^2 \pi^2 D_i t}{x_e^2}\right) (-1)^n \cos\left(\frac{n\pi x}{x_e}\right) \right] \quad (4.37)$$

The solution for the change in concentration of a component at a given point x and time t is then obtained by numerical integration of equation (4.35), with the source functions given by equations (4.36) and (4.37).

4.3.4. LAPLACE DOMAIN SOLUTION

4.3.4.1. Infinite Media Source Function

From equation (4.25), the differential equation to be solved for the source function will be given by:

$$D_i \frac{\partial^2 \bar{G}(x,s)}{\partial x^2} - s\bar{G}(x,s) = 0 \quad (4.38)$$

The solution of this equation is performed in an identical manner to the time domain solution, as the Laplace transform was used in that case and the result subjected to the inverse transform to obtain the function given in equation (4.28). The boundary conditions used to obtain this solution are given as:

$$\begin{aligned}\overline{G}(x,s)\Big|_{x=\infty} &= 0 \\ \frac{\partial \overline{G}(x,s)}{\partial x}\Big|_{x=0} &= -\frac{1}{D_i s}\end{aligned}\tag{4.39}$$

and the Laplace space source function for a one-dimensional infinite region with an infinite plane source located at x' that results is:

$$\overline{G}(x,x',s) = \frac{1}{2\sqrt{D_i s}} \exp\left[-|x-x'|\sqrt{s/D_i}\right]$$

4.3.4.2. Bounded Media Source Function

The source function for the bounded media can also be derived using the method of images employed for the time domain solution. A simpler method is presented by van Kruijsdijk and Dullaert (1989), in which the equation given in (4.38) is solved over two regions:

$$\begin{aligned}\overline{G} &= \begin{cases} \overline{G}_l & 0 \leq x \leq x' \\ \overline{G}_r & x' \leq x \leq x_e \end{cases} \\ \overline{G}_l\Big|_{x=x'} &= \overline{G}_r\Big|_{x=x'}\end{aligned}\tag{4.40}$$

subject to the following boundary conditions:

$$\begin{aligned}\frac{\partial \overline{G}_l(x,s)}{\partial x}\Big|_{x=0} &= \frac{\partial \overline{G}_r(x,s)}{\partial x}\Big|_{x=x_e} = 0 \\ \frac{\partial \overline{G}_l(x,s)}{\partial x}\Big|_{x=x'} &- \frac{\partial \overline{G}_r(x,s)}{\partial x}\Big|_{x=x'} = \frac{1}{D_i s}\end{aligned}\tag{4.41}$$

This results in the source function for a finite one-dimensional domain with no-flow boundaries at $x = 0$ and $x = x_e$ and a source at point x' as follows:

$$\begin{aligned} \bar{G}(x, x', s) = \frac{1}{2\sqrt{D_i s}} \left\{ \frac{2 \cosh[(x - x')\sqrt{s/D_i}]}{\exp(2x_e\sqrt{s/D_i}) - 1} + \exp[-|x - x'|\sqrt{s/D_i}] \right. \\ \left. + \frac{2 \cosh[(x + x')\sqrt{s/D_i}]}{\exp(2x_e\sqrt{s/D_i}) - 1} + \exp[-|x + x'|\sqrt{s/D_i}] \right\} \end{aligned} \quad (4.42)$$

This result and a number of other source functions in Laplace space for reservoir problems in one, two, and three dimensions are given by van Kruijsdijk (1988).

4.3.4.3. Application of the Integral Equation

The integral equation for solution in the Laplace domain is shown in equation (4.19). Again proceeding as for the time domain solution, the boundary integral over the source domain reduces to the summation of two terms: one with the source function positioned at $x' = 0$, and the other with the source function positioned at $x = x_e$. The final equation for generation of the one-dimensional concentration gradient in Laplace space is given by

$$\Delta \bar{\rho}_i(x, s) = \bar{f}(s) \bar{G}(x, x' = 0, s) + \bar{g}(s) \bar{G}(x, x' = x_e, s) \quad (4.43)$$

with the source functions defined as follows:

$$\bar{G}(x, x' = 0, s) = \frac{\exp[x\sqrt{s/D_i}] + \exp[(2x_e - x)\sqrt{s/D_i}]}{\sqrt{D_i s} [\exp(2x_e\sqrt{s/D_i}) - 1]} \quad (4.44)$$

$$\bar{G}(x, x' = x_e, s) = \frac{\exp[(x_e + x)\sqrt{s/D_i}] + \exp[(x_e - x)\sqrt{s/D_i}]}{\sqrt{D_i s} [\exp(2x_e\sqrt{s/D_i}) - 1]} \quad (4.45)$$

The solution for the change in concentration at any point x and for any value of s may be obtained directly by substituting the Laplace transformed values of the flux functions into equation (4.43), with the source functions given by equations (4.44) and (4.45).

4.3.5. EXTENSION AND EVALUATION

Some elaborations on Green's function methods for solving the diffusion equation with prescribed flux boundary conditions are presented in the Appendix. The Appendix includes details on the Laplace domain solution procedure for one-dimensional problems, an extension of the principal equations to two-dimensional problems and some numerical examples developed to evaluate the usefulness of the time domain and Laplace domain solution procedures with some model flux functions.

4.4. SOLUTION OF THE DIFFUSION EQUATION WITH LINEAR INITIAL CONDITIONS

4.4.1. INTEGRAL EQUATION FORMULATION

For problems in the infinite domain or in domains with impermeable boundaries, assuming no source/sink terms, the concentration response at any time will depend only on the initial concentration distribution. For these situations, the solution of the diffusion equation (4.5) given in integral form in equation (4.15) will reduce to

$$\rho_i(\mathbf{x}, t) = \iiint \rho_i(\mathbf{x}', t = 0) G(\mathbf{x}, \mathbf{x}', t) d\mathbf{x}' \quad (4.46)$$

The source function G is found in the same manner as for the infinite and bounded cases for the prescribed flux boundary conditions. The evaluation of this integral for various linear initial conditions is shown in the following sections. The derivation of analytical forms for the concentration distribution has the advantage that closed forms for concentration gradients and integrals of the concentration in space may be evaluated for the determination of diffusive flux in reservoir simulators with minimal computational effort.

Solutions of the diffusion equation for infinite and bounded cases have been found by various methods including separation of variables, Laplace transforms and expansion of trigonometric series. Carslaw and Jaeger (1959) and Crank (1975) give solutions for single step function initial conditions; the form of solutions for general initial condition functions are also shown. Again, the Green's function formulation is used here to provide a single methodology for the derivation of solutions for a number of initial conditions.

4.4.2. SOLUTION OF THE CONCENTRATION DIFFUSION EQUATION IN ONE DIMENSION

4.4.2.1. Infinite Medium, Step Function Initial Condition

The diffusion equation will be solved under the following initial condition:

$$\begin{aligned}\rho_i(x, t=0) &= \rho_{i,1} & x < x_1 \\ \rho_i(x, t=0) &= \rho_{i,2} & x > x_1\end{aligned}\quad (4.47)$$

The infinite media source function given in equation (4.28) will be used, thus equation (4.46) can be written

$$\rho_i(x, t) = \int_{-\infty}^{x_1} \rho_{i,1} \frac{\exp[-(x-x')^2/4D_i t]}{2\sqrt{\pi D_i t}} dx' + \int_{x_1}^{\infty} \rho_{i,2} \frac{\exp[-(x-x')^2/4D_i t]}{2\sqrt{\pi D_i t}} dx' \quad (4.48)$$

The solution to this equation is obtained by letting

$$\eta = (x - x') / 2\sqrt{D_i t} \quad (4.49)$$

and rewriting equation (4.48) as:

$$\rho_i(x, t) = \frac{\rho_{i,1}}{2\sqrt{\pi D_i t}} \int_{\frac{x-x_1}{2\sqrt{D_i t}}}^{\infty} \exp(-\eta^2) d\eta - \frac{\rho_{i,2}}{2\sqrt{\pi D_i t}} \int_{\frac{x-x_1}{2\sqrt{D_i t}}}^{\infty} \exp(-\eta^2) d\eta \quad (4.50)$$

Using the following relation with the error function

$$\begin{aligned} \frac{2}{\sqrt{\pi}} \int_z^{\infty} \exp(-\eta^2) d\eta &= \frac{2}{\sqrt{\pi}} \int_0^{\infty} \exp(-\eta^2) d\eta - \frac{2}{\sqrt{\pi}} \int_0^z \exp(-\eta^2) d\eta \\ &= 1 - \operatorname{erf}(z) = \operatorname{erfc}(z) \end{aligned} \quad (4.51)$$

gives the final result for the concentration profile:

$$\rho_i(x, t) = \rho_{i,2} + \frac{\rho_{i,1} - \rho_{i,2}}{2} \operatorname{erfc}\left(\frac{x - x_1}{2\sqrt{D_i t}}\right) \quad (4.52)$$

This is the well known error function form of the solution to the diffusion equation. Integrals and derivatives of the error function are given in Carslaw and Jaeger (1959; p. 484). Repeated integrals are evaluated with the following recurrence formula:

$$2ni^n \operatorname{erfc}x = i^{n-2} \operatorname{erfc}x - 2xi^{n-1} \operatorname{erfc}x \quad (4.53)$$

where:

$$\begin{aligned} i^n \operatorname{erfc}x &= \int_x^{\infty} i^{n-1} \operatorname{erfc}\xi d\xi \quad ; \quad n = 1, 2, \dots \\ i^0 \operatorname{erfc}x &= \operatorname{erfc}x \\ i \operatorname{erfc}x &= \frac{1}{\sqrt{\pi}} e^{-x^2} - x \operatorname{erfc}x \end{aligned} \quad (4.54)$$

Derivatives are defined simply by:

$$\begin{aligned} \Phi_n(x) &= \frac{d^n}{dx^n} \operatorname{erfc}x \\ \Phi_1(x) &= \frac{2}{\sqrt{\pi}} e^{-x^2} \\ \Phi_2(x) &= -\frac{4}{\sqrt{\pi}} x e^{-x^2} \quad , \quad \text{etc.} \end{aligned} \quad (4.55)$$

Application of these rules allows the concentration gradient to be expressed as:

$$\frac{\partial \rho_i(x, t)}{\partial x} = -\frac{\rho_{i,1} - \rho_{i,2}}{2\sqrt{\pi D_i t}} \exp\left[-(x - x_1)^2 / 4D_i t\right] \quad (4.56)$$

The number of moles of component i in any section of the domain may be determined by integration of the profile, resulting in:

$$\begin{aligned}
\int_{x_a}^{x_b} \rho_i(x, t) dx &= \rho_{i,2}(x_b - x_a) + \frac{\rho_{i,1} - \rho_{i,2}}{2} \\
&\cdot \left[\left[2\sqrt{D_i t} / \pi \exp(-(x_a - x_1)^2 / 4D_i t) - (x_a - x_1) \operatorname{erfc}((x_a - x_1) / 2\sqrt{D_i t}) \right] \right. \\
&\quad \left. - \left[2\sqrt{D_i t} / \pi \exp(-(x_b - x_1)^2 / 4D_i t) - (x_b - x_1) \operatorname{erfc}((x_b - x_1) / 2\sqrt{D_i t}) \right] \right] \quad (4.57)
\end{aligned}$$

4.4.2.2. Bounded Medium, Step Function Initial Condition

In this section, a special case in which the step is located at the midpoint of the bounded region is considered. A more general condition involving multiple step functions is considered later. The initial condition is given by:

$$\begin{aligned}
\rho_i(x, t=0) &= \rho_{i,1} & 0 \leq x < \Delta x / 2 \\
\rho_i(x, t=0) &= \rho_{i,2} & \Delta x / 2 < x \leq \Delta x
\end{aligned} \quad (4.58)$$

The bounded media source function is the one given in equation (4.34). Integration of this source function according to equation (4.46) yields the following formula for the concentration profile:

$$\begin{aligned}
\rho_i(x, t) &= \frac{\rho_{i,1} + \rho_{i,2}}{2} \\
&+ \frac{2(\rho_{i,1} - \rho_{i,2})}{\pi} \sum_{n=1}^{\infty} \frac{(-1)^{n-1}}{2n-1} \exp\left(\frac{-(2n-1)^2 \pi^2 D_i t}{\Delta x^2}\right) \cos\left(\frac{(2n-1)\pi x}{\Delta x}\right) \quad (4.59)
\end{aligned}$$

The concentration gradient will be given by

$$\frac{\partial \rho_i(x, t)}{\partial x} = -\frac{2(\rho_{i,1} - \rho_{i,2})}{\Delta x} \sum_{n=1}^{\infty} (-1)^{n-1} \exp\left(\frac{-(2n-1)^2 \pi^2 D_i t}{\Delta x^2}\right) \sin\left(\frac{(2n-1)\pi x}{\Delta x}\right) \quad (4.60)$$

and the integral of the profile is:

$$\begin{aligned}
\int_{x_a}^{x_b} \rho_i(x, t) dx &= \frac{\rho_{i,1} + \rho_{i,2}}{2} (x_a - x_b) + \frac{2\Delta x (\rho_{i,1} - \rho_{i,2})}{\pi^2} \\
&\cdot \sum_{n=1}^{\infty} \frac{(-1)^{n-1}}{2n-1} \exp\left(\frac{-(2n-1)^2 \pi^2 D_i t}{\Delta x^2}\right) \left[\sin\left(\frac{(2n-1)\pi x_b}{\Delta x}\right) - \sin\left(\frac{(2n-1)\pi x_a}{\Delta x}\right) \right] \quad (4.61)
\end{aligned}$$

As was discussed in the comparison of Laplace and time domain solution procedures, the infinite series present in the bounded media source functions for the time domain can converge very slowly for small values of time. It is possible that a Laplace solution of the above problem may be advantageous, however, numerical inversion of the transformed equation requires at least 8 evaluations of the Laplace domain equation to generate a result for one time value. The Laplace domain solution is shown in this case only to allow a comparison of the time domain and Laplace domain solutions.

The Laplace domain source function for bounded media is the one given in equation (4.42). The resulting concentration profile in Laplace space is:

$$\bar{\rho}_i(x, s) = \frac{\rho_{i,1} + \rho_{i,2}}{2s} + \frac{\rho_{i,1} - \rho_{i,2}}{2s} \left\{ \begin{aligned} & -\frac{x - \Delta x/2}{|x - \Delta x/2|} \left[1 - \exp(-|x - \Delta x/2|\sqrt{s/D_i}) \right] - \exp(-|x + \Delta x/2|\sqrt{s/D_i}) \\ & + \frac{-2 \sinh((x - \Delta x/2)\sqrt{s/D_i}) + 2 \sinh((x + \Delta x/2)\sqrt{s/D_i})}{\exp(2\Delta x\sqrt{s/D_i}) - 1} \end{aligned} \right\} \quad (4.62)$$

with the concentration gradient given by

$$\frac{\partial \bar{\rho}_i(x, s)}{\partial x} = \frac{\rho_{i,1} - \rho_{i,2}}{2\sqrt{sD_i}} \left\{ \begin{aligned} & \exp(-|x + \Delta x/2|\sqrt{s/D_i}) - \exp(-|x - \Delta x/2|\sqrt{s/D_i}) \\ & + \frac{-2 \cosh((x - \Delta x/2)\sqrt{s/D_i}) + 2 \cosh((x + \Delta x/2)\sqrt{s/D_i})}{\exp(2\Delta x\sqrt{s/D_i}) - 1} \end{aligned} \right\} \quad (4.63)$$

and the integral of the profile is:

$$\begin{aligned}
\int_{x_a}^{x_b} \bar{\rho}_i(x, s) dx &= \frac{\rho_{i,2}}{s} (x_b - x_a) + \frac{\rho_{i,1} - \rho_{i,2}}{2\sqrt{s^3 / D_i}} \\
&\cdot \left\{ \begin{aligned} & -\exp(-|x_b - \Delta x/2|\sqrt{s / D_i}) + \exp(-|x_b + \Delta x/2|\sqrt{s / D_i}) \\ & + \exp(-|x_a - \Delta x/2|\sqrt{s / D_i}) - \exp(-|x_a + \Delta x/2|\sqrt{s / D_i}) \\ & - 2\cosh((x_b - \Delta x/2)\sqrt{s / D_i}) + 2\cosh((x_b + \Delta x/2)\sqrt{s / D_i}) \\ & + \frac{\exp(2\Delta x\sqrt{s / D_i}) - 1}{-2\cosh((x_a - \Delta x/2)\sqrt{s / D_i}) + 2\cosh((x_a + \Delta x/2)\sqrt{s / D_i})} \\ & - \frac{\exp(2\Delta x\sqrt{s / D_i}) - 1}{-2\cosh((x_a - \Delta x/2)\sqrt{s / D_i}) + 2\cosh((x_a + \Delta x/2)\sqrt{s / D_i})} \end{aligned} \right\}
\end{aligned} \tag{4.64}$$

4.4.2.3. Infinite Medium, Multiple Step Function Initial Condition

This solution may be used for situations in which the initial condition can be approximated as a number of zero order (horizontal) linear segments of arbitrary length.

The initial condition will be expressed as:

$$\begin{aligned}
\rho_i(x, t = 0) &= \rho_{i,1} & -\infty < x < x_1 \\
\rho_i(x, t = 0) &= \rho_{i,2} & x_1 < x < x_2 \\
&\vdots & \vdots \\
\rho_i(x, t = 0) &= \rho_{i,m} & x_{m-1} < x < x_m \\
&\vdots & \vdots \\
\rho_i(x, t = 0) &= \rho_{i,N} & x_{N-1} < x < \infty
\end{aligned} \tag{4.65}$$

Performing the integration of equation (4.46) under these conditions with the infinite media source function gives the following expression for the concentration profile:

$$\rho_i(x, t) = \rho_{i,N} + \sum_{m=1}^{N-1} \frac{\rho_{i,m} - \rho_{i,m+1}}{2} \operatorname{erfc}\left(\frac{x - x_m}{2\sqrt{D_i t}}\right) \tag{4.66}$$

The expressions for the concentration gradient and integral of the profile will be given by:

$$\frac{\partial \rho_i(x, t)}{\partial x} = - \sum_{m=1}^{N-1} \frac{\rho_{i,m} - \rho_{i,m+1}}{2\sqrt{\pi D_i t}} \exp\left[-(x - x_m)^2 / 4D_i t\right] \quad (4.67)$$

$$\int_{x_a}^{x_b} \rho_i(x, t) dx = \rho_{i,N}(x_b - x_a) + \sum_{m=1}^{N-1} \frac{\rho_{i,m} - \rho_{i,m+1}}{2} \left\{ 2\sqrt{D_i t / \pi} \left[\exp\left(-(x_a - x_m)^2 / 4D_i t\right) - \exp\left(-(x_b - x_m)^2 / 4D_i t\right) \right] + (x_b - x_m) \operatorname{erfc}\left(\frac{x_b - x_m}{2\sqrt{D_i t}}\right) - (x_a - x_m) \operatorname{erfc}\left(\frac{x_a - x_m}{2\sqrt{D_i t}}\right) \right\} \quad (4.68)$$

4.4.2.4. Bounded Medium, Multiple Step Function Initial Condition

The multiple step function with impermeable boundaries at $x=0$ and $x=x_N$ is described by the initial condition

$$\begin{aligned} \rho_i(x, t=0) &= \rho_{i,1} & 0 < x < x_1 \\ \rho_i(x, t=0) &= \rho_{i,2} & x_1 < x < x_2 \\ &\vdots & \vdots \\ \rho_i(x, t=0) &= \rho_{i,m} & x_{m-1} < x < x_m \\ &\vdots & \vdots \\ \rho_i(x, t=0) &= \rho_{i,N} & x_{N-1} < x < x_N \end{aligned} \quad (4.69)$$

The resulting concentration profile is:

$$\rho_i(x, t) = \rho_{i,N} + \sum_{m=1}^{N-1} (\rho_{i,m} - \rho_{i,m+1}) \left[\frac{x_m}{x_N} + \frac{2}{\pi} \sum_{n=1}^{\infty} \frac{1}{n} \exp\left(\frac{-n^2 \pi^2 D_i t}{x_N^2}\right) \cos\left(\frac{n\pi x}{x_N}\right) \sin\left(\frac{n\pi x_m}{x_N}\right) \right] \quad (4.70)$$

The concentration gradient will be

$$\frac{\partial \rho_i(x, t)}{\partial x} = - \frac{2}{x_N} \sum_{m=1}^{N-1} (\rho_{i,m} - \rho_{i,m+1}) \sum_{n=1}^{\infty} \exp\left(\frac{-n^2 \pi^2 D_i t}{x_N^2}\right) \cos\left(\frac{n\pi x}{x_N}\right) \sin\left(\frac{n\pi x_m}{x_N}\right) \quad (4.71)$$

and the integral of the profile is given by

$$\begin{aligned}
\int_{x_a}^{x_b} \rho_i(x, t) dx &= \rho_{i,N}(x_b - x_a) + \sum_{m=1}^{N-1} (\rho_{i,m} - \rho_{i,m+1}) \left\{ \frac{x_m}{x_N} (x_b - x_a) \right. \\
&\quad \left. + \frac{2x_N}{\pi^2} \sum_{n=1}^{\infty} \frac{1}{n^2} \exp\left(\frac{-n^2 \pi^2 D_i t}{x_N^2}\right) \sin\left(\frac{n\pi x_m}{x_N}\right) \left[\sin\left(\frac{n\pi x_b}{x_N}\right) - \sin\left(\frac{n\pi x_a}{x_N}\right) \right] \right\}
\end{aligned} \tag{4.72}$$

4.4.2.5. Infinite Medium, Piecewise Linear Function Initial Condition

This solution may be used for situations in which the initial condition can be approximated as a number of linear segments of arbitrary length. The initial condition will be expressed as:

$$\begin{aligned}
\rho_i(x, t=0) &= \rho_{i,1} & -\infty < x \leq x_1 \\
\rho_i(x, t=0) &= \rho_{i,1} + S_1(x - x_1) & x_1 < x \leq x_2 \\
&\vdots & \vdots \\
\rho_i(x, t=0) &= \rho_{i,m} + S_m(x - x_m) & x_m < x \leq x_{m+1} \\
&\vdots & \vdots \\
\rho_i(x, t=0) &= \rho_{i,N-1} + S_{N-1}(x - x_{N-1}) & x_{N-1} < x \leq x_N \\
\rho_i(x, t=0) &= \rho_{i,N} & x_N < x < \infty
\end{aligned}$$

where $S_m = \frac{\rho_{i,m} - \rho_{i,m+1}}{x_m - x_{m+1}}$

(4.73)

The concentration profile resulting from this initial condition is:

$$\begin{aligned}
\rho_i(x, t) &= \frac{\rho_{i,1} + \rho_{i,N}}{2} - \\
&\sum_{m=1}^N \left\{ \frac{1}{2} [(\rho_{i,m-1} + S_{m-1}(x - x_{m-1})) - (\rho_{i,m} + S_m(x - x_m))] \operatorname{erf}\left(\frac{x - x_m}{2\sqrt{D_i t}}\right) \right. \\
&\quad \left. + (S_{m-1} - S_m) \sqrt{D_i t / \pi} \exp[-(x - x_m)^2 / 4D_i t] \right\}
\end{aligned} \tag{4.74}$$

The concentration gradient will be expressed as:

$$\frac{\partial \rho_i(x, t)}{\partial x} = - \sum_{m=1}^N \left\{ \frac{(\rho_{i,m-1} - \rho_{i,m}) - S_{m-1}(x_{m-1} - x_m)}{2\sqrt{\pi D_i t}} \exp\left[-(x - x_m)^2 / 4D_i t\right] + \frac{(S_{m-1} - S_m)}{2} \operatorname{erf}\left(\frac{x - x_m}{2\sqrt{D_i t}}\right) \right\} \quad (4.75)$$

and the integration, again using the recurrence formulas for the error function, results in the following:

$$\begin{aligned} \int_{x_a}^{x_b} \rho_i(x, t) dx &= \frac{\rho_{i,1} + \rho_{i,N}}{2} (x_b - x_a) + \frac{1}{2} \sum_{m=1}^N \left\{ [(\rho_{i,m-1} - \rho_{i,m}) + S_{m-1}(x_m - x_{m-1})] \right. \\ &\cdot \left[\left(2\sqrt{D_i t / \pi} \exp\left[-(x_a - x_m)^2 / 4D_i t\right] - (x_a - x_m) \operatorname{erfc}\left(\frac{x_a - x_m}{2\sqrt{D_i t}}\right) \right) \right. \\ &- \left. \left(2\sqrt{D_i t / \pi} \exp\left[-(x_b - x_m)^2 / 4D_i t\right] - (x_b - x_m) \operatorname{erfc}\left(\frac{x_b - x_m}{2\sqrt{D_i t}}\right) \right) \right] - (S_{m-1} - S_m) \\ &\cdot \left[\left((D_i t + (x_a - x_m)^2 / 2) \operatorname{erfc}\left(\frac{x_a - x_m}{2\sqrt{D_i t}}\right) - \sqrt{D_i t / \pi} (x_a - x_m) \exp\left[-(x_a - x_m)^2 / 4D_i t\right] \right) \right. \\ &- \left. \left((D_i t + (x_b - x_m)^2 / 2) \operatorname{erfc}\left(\frac{x_b - x_m}{2\sqrt{D_i t}}\right) - \sqrt{D_i t / \pi} (x_b - x_m) \exp\left[-(x_b - x_m)^2 / 4D_i t\right] \right) \right] \\ &\left. - (\rho_{i,m-1} - \rho_{i,m} + S_m x_m - S_{m-1} x_{m-1})(x_b - x_a) - \frac{(S_{m-1} - S_m)}{2} (x_b^2 - x_a^2) \right\} \end{aligned} \quad (4.76)$$

4.4.2.6. Bounded Medium, Piecewise Linear Function Initial Condition

The piecewise linear function with impermeable boundaries at $x = 0$ and $x = x_{N+1}$ is described by the initial condition:

$$\begin{aligned}
\rho_i(x, t=0) &= \rho_{i,1} & 0 < x \leq x_1 \\
\rho_i(x, t=0) &= \rho_{i,1} + S_1(x - x_1) & x_1 < x \leq x_2 \\
&\vdots & \vdots \\
\rho_i(x, t=0) &= \rho_{i,m} + S_m(x - x_m) & x_m < x \leq x_{m+1} \\
&\vdots & \vdots \\
\rho_i(x, t=0) &= \rho_{i,N-1} + S_{N-1}(x - x_{N-1}) & x_{N-1} < x \leq x_N \\
\rho_i(x, t=0) &= \rho_{i,N} & x_N < x < x_{N+1}
\end{aligned}$$

where $S_m = \frac{\rho_{i,m} - \rho_{i,m+1}}{x_m - x_{m+1}}$

(4.77)

The concentration profile in this case will be:

$$\begin{aligned}
\rho_i(x, t) &= \frac{\rho_{i,1}x_1}{x_{N+1}} + \sum_{m=1}^N \left\{ \frac{S_m}{x_{N+1}} \left(\frac{x_m^2 + x_{m+1}^2}{2} - x_m x_{m+1} \right) + \frac{\rho_{i,m}}{x_{N+1}} (x_{m+1} - x_m) \right. \\
&+ 2 \sum_{n=1}^{\infty} \left[\frac{1}{n\pi} \exp\left(\frac{-n^2 \pi^2 D_i t}{x_{N+1}^2} \right) \cos\left(\frac{n\pi x}{x_{N+1}} \right) \right] \\
&\left. \left[\left((\rho_{i,m-1} - \rho_{i,m}) + S_{m-1}(x_m - x_{m-1}) \right) \sin\left(\frac{n\pi x_m}{x_{N+1}} \right) - \frac{x_{N+1}}{n\pi} (S_m - S_{m-1}) \cos\left(\frac{n\pi x_m}{x_{N+1}} \right) \right] \right\}
\end{aligned}$$

(4.78)

Resulting in the following formulas for concentration gradient

$$\begin{aligned}
\frac{\partial \rho_i(x, t)}{\partial x} &= \frac{-2}{x_{N+1}} \sum_{m=1}^N \left\{ \sum_{n=1}^{\infty} \left[\exp\left(\frac{-n^2 \pi^2 D_i t}{x_{N+1}^2} \right) \sin\left(\frac{n\pi x}{x_{N+1}} \right) \right] \right. \\
&\left. \left[\left((\rho_{i,m-1} - \rho_{i,m}) + S_{m-1}(x_m - x_{m-1}) \right) \sin\left(\frac{n\pi x_m}{x_{N+1}} \right) - \frac{x_{N+1}}{n\pi} (S_m - S_{m-1}) \cos\left(\frac{n\pi x_m}{x_{N+1}} \right) \right] \right\}
\end{aligned}$$

(4.79)

and integral:

$$\begin{aligned}
\int_{x_a}^{x_b} \rho_i(x, t) dx &= \frac{\rho_{i,1} x_1}{x_{N+1}} (x_b - x_a) \\
&+ \sum_{m=1}^N \left\{ \left[\frac{S_m}{x_{N+1}} \left(\frac{x_m^2 + x_{m+1}^2}{2} - x_m x_{m+1} \right) + \frac{\rho_{i,m}}{x_{N+1}} (x_{m+1} - x_m) \right] (x_b - x_a) \right. \\
&+ 2 \sum_{n=1}^{\infty} \left[\frac{x_{N+1}}{n^2 \pi^2} \exp \left(\frac{-n^2 \pi^2 D_i t}{x_{N+1}^2} \right) \right] \left[\sin \left(\frac{n \pi x_b}{x_{N+1}} \right) - \sin \left(\frac{n \pi x_a}{x_{N+1}} \right) \right] \\
&\left. \cdot \left[\left((\rho_{i,m-1} - \rho_{i,m}) + S_{m-1} (x_m - x_{m-1}) \right) \sin \left(\frac{n \pi x_m}{x_{N+1}} \right) - \frac{x_{N+1}}{n \pi} (S_m - S_{m-1}) \cos \left(\frac{n \pi x_m}{x_{N+1}} \right) \right] \right\}
\end{aligned}$$

(4.80)

4.4.3. CONCENTRATION PROFILES FROM MULTIPLE STEP AND PIECEWISE LINEAR INITIAL CONDITIONS

One possible application of the concentration profile solutions in the infinite domain for the multiple step and piecewise linear initial conditions is illustrated in this section. The solutions are generated by first selecting the number of segments to be used, then generating a profile to be used as an initial condition. In this case, the initial condition will be given by the error function solution of the diffusion equation given in equation (4.52). Use of this function will allow "exact" solutions to be generated at any desired time to compare to the results obtained with the approximate initial conditions.

The approximate initial conditions are determined by first integrating the initial profile over each segment of the domain, using equation (4.57), to obtain an average concentration for each segment. For the multiple step solution, the initial concentration is assumed to be constant and equal to this average for each segment; for the piecewise linear solution, the initial condition is given by chords connecting the midpoint of each segment, with the nodes defined by the average concentrations. The solutions corresponding to these initial conditions can then be generated using equation (4.66) for the multiple step initial condition, and equation (4.74) for the piecewise linear condition, for any value of time.

In Figure 4.3 the results for the region $0 < x_D < 1$ are shown for an initial profile generated from a step positioned at $x_D = 0.5$. This region is divided into 6 segments for the

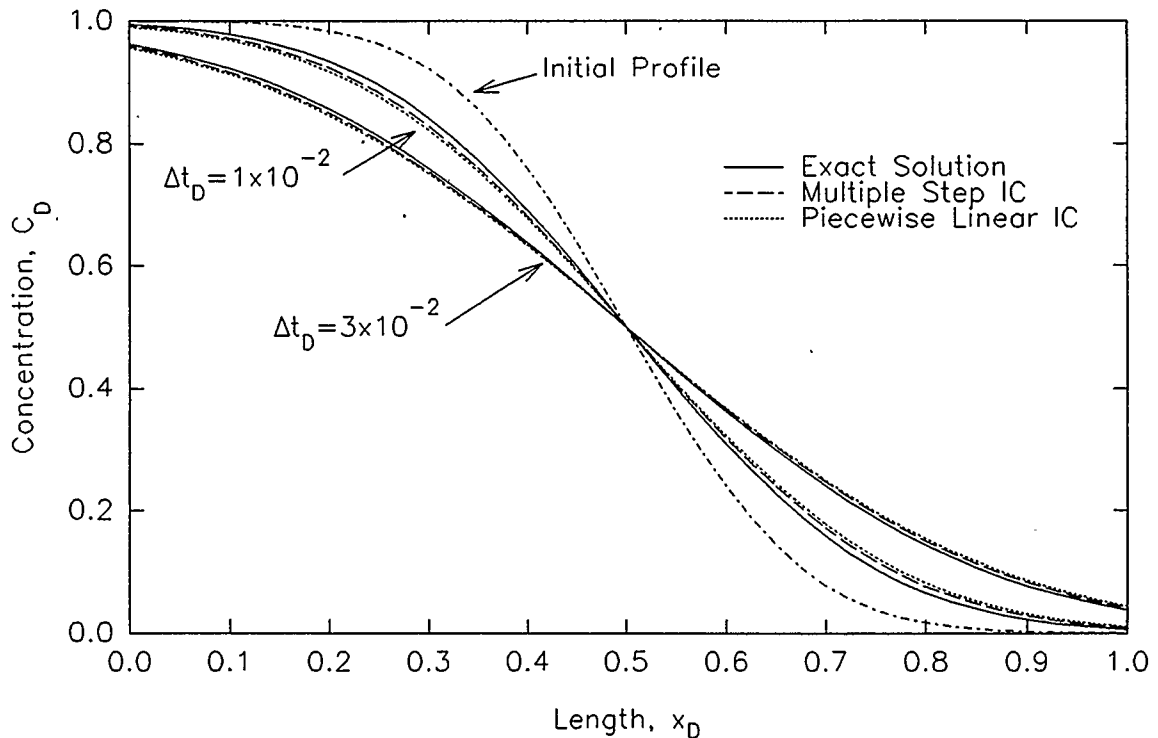


Figure 4.3: Concentration Profiles from Linear Initial Conditions, 6 Segments

approximate initial condition definition. Profiles calculated at two values of elapsed time are shown for the multiple step and piecewise linear solutions. The results shown here indicate that good agreement to the exact solutions can be achieved using approximate initial conditions, even when only a small number of linear segments are used. In this case it is also apparent that the two approximate methods provide almost identical results.

These solutions may also be used for cases in which the parameters in the diffusion equation change with time, or when the profile is shaped by forces other than diffusion. In these situations, rather than generating a number of solutions at various times from a single initial condition, the approximate initial condition can be re-evaluated before each time step; this initial condition can reflect the influence of forces other than diffusion, and different parameters can be used in the generation of the next profile.

To simulate a situation of this type, the solution procedure outlined above is modified to allow recalculation of an approximate initial condition after each time step. This is done simply by integrating the profiles generated using the multiple step and piecewise linear solutions over each segment, as was done in the initiation step described above. In this case the integrals are defined by equation (4.68) for the multiple step solution and equation (4.76) for the piecewise linear solution.

In Figure 4.4, the results of this calculation are shown for the same six segment case discussed above. The time step size used is $\Delta t_D = 1 \times 10^{-2}$. The result after one time step is of course the same as that shown in Figure 4.3; after three time steps the solutions have started to diverge slightly, although the agreement is still very good. The piecewise linear solution shows somewhat more spread than the multiple step solution.

The results shown in these figures indicate that very good representations of the diffusion profile may be calculated from simple stepwise linear approximations of the initial condition.

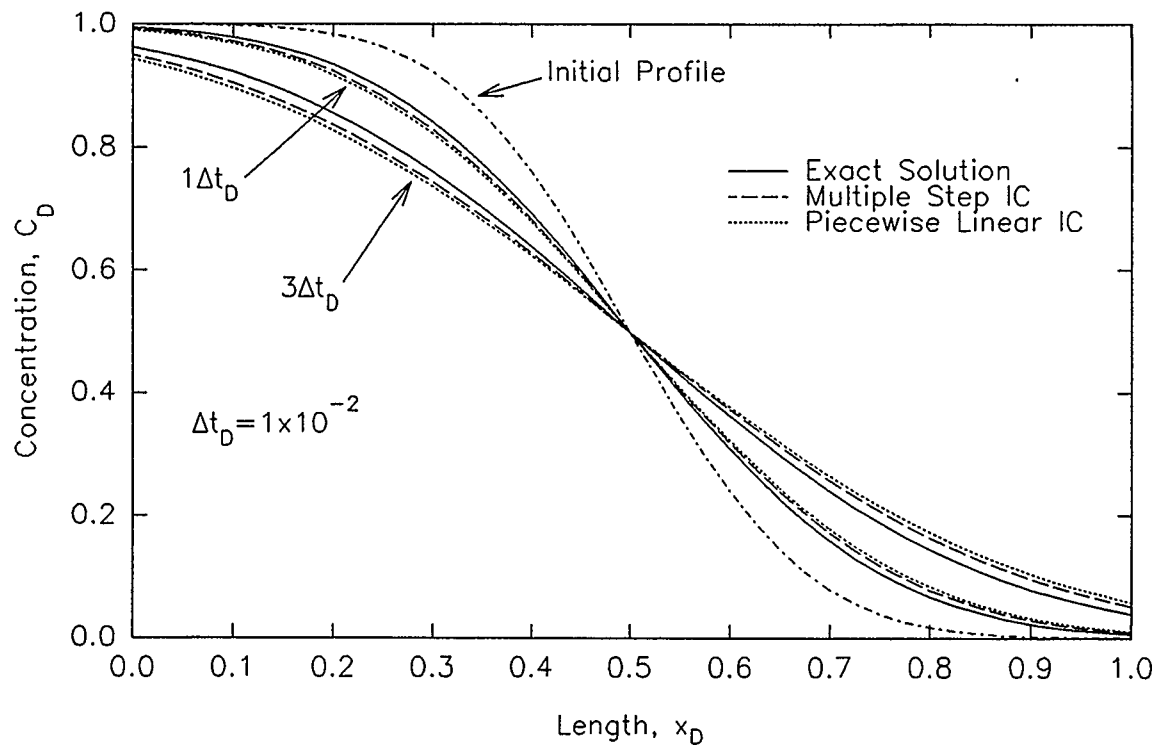


Figure 4.4: Concentration Profiles with Initial Condition Re-Evaluation, 6 Segments, $\Delta t_D = 1 \times 10^{-2}$

5. IMPLEMENTATION OF DISPERSIVE FLUX MODELS IN THE COMPOSITIONAL SIMULATOR

In this chapter, the methods for implementing Fick's first law and the solutions of Fick's second law for determination of dispersive flux in the compositional model are developed. The fundamental method for incorporating dispersion into the simulator used for all of the models is the addition of dispersive flow rates as source/sink terms in the convective flow equation. Thus, each dispersion model can be programmed as a separate module, and a single main reservoir simulation model calls the desired dispersion subroutine when the source/sink terms must be generated. The steps in the algorithms for the two-dimensional application of the first law model and the approximate initial condition form of the second law model are given here. The front tracking model utilizing the second law solutions is also developed but for use in only one dimension.

5.1. FICK'S FIRST LAW MODEL

The Fick's first law model for dispersion developed here follows a diffusive flux model presented by Thiebot and Sakthikumar (1991). The form of the first law shown in equation (4.3) is used here, with an effective dispersion coefficient for each component in the multicomponent system. The dispersive flux terms are evaluated explicitly, that is from the conditions existing at the beginning of a time step, and are included as source or sink terms in the convective flow equations. A schematic diagram of the conditions existing at the beginning of a time step for any two grid blocks is shown below in Figure 5.1.

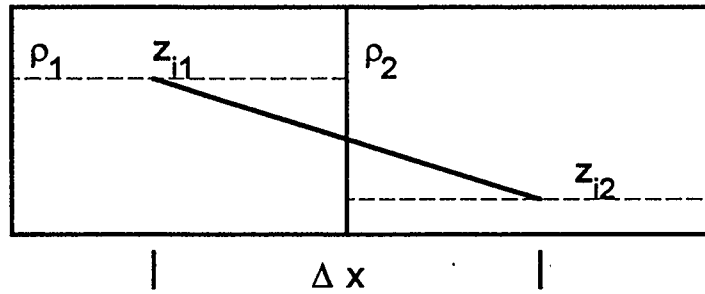


Figure 5.1: First Law Model Schematic

The concentration gradient across the interface driving the dispersive flux is defined as the difference in mole fraction of a given component between the two grid blocks over the distance between the midpoints of the blocks. A constant value of the global molar density must be used in the first law equation; for this model the harmonic mean of the molar densities in the two grid blocks is used as follows:

$$\rho_{avg} = \frac{2\rho_1\rho_2}{\rho_1 + \rho_2} \quad (5.1)$$

Applying the above definitions for concentration gradient and average density with equation (4.3) results in the molar flux (kmol/m²s) of a component across the interface being given by

$$j_i = \rho_{avg} D_i \frac{\Delta z_i}{\Delta x} \quad (5.2)$$

This flux is converted to a molar flow rate simply by multiplying it by the area available for flow across the interface, giving the following equation for molar dispersive flow rate:

$$q_{d,i} = A \phi \rho_{avg} D_i \frac{\Delta z_i}{\Delta x} \quad (5.3)$$

Should the two grid blocks have different values of porosity, a harmonic average can again be used.

This value for molar flow rate is applied as a source for the block which has the lower mole fraction of the component, and as a sink for the block with the higher mole

fraction. Thus, the dispersive component molar flow rate for a given grid block will be equal to the sum of the dispersive component flow rates across each grid block face. The total component source or sink rate is obtained by summing the dispersive rate with any well sources or sinks of that component present in the grid block as shown in equation (3.57). This total component source/sink is used in equation (3.73) for solution of the composition in a grid block. The sum of the component flow rates for a given grid block gives the total molar flow rate to be used in the solution of the pressure equation given in equation (3.62).

The advantages of this First law model are that it is easy to implement in a conventional simulator, and may be applied for problems in one, two or three dimensions. The structure of the matrix for solution of the pressure equation does not change, and any methods for numerical dispersion control will not be affected. As the dispersive flow rates are defined as constants at the start of the time step and have zero derivatives with respect to pressure, they do not appear in the Jacobian for the pressure equation solution. The accuracy of the dispersive flux predicted by the model will depend on a number of parameters. The size of the grid blocks in the simulation model will affect the slope of the concentration gradient defining the driving force for the dispersive flux. A finer grid will be subject to lower levels of numerical dispersion, and will result in inter-block gradients that model the physical concentration profiles present in the reservoir more closely than those resulting from a coarse grid. Numerical dispersion is also minimized by using the maximum time step size, up to the stability limit imposed by the throughput condition.

The model formulation assumes that the inter-block gradients remain constant over a time step. For small time steps and small values of the dispersion coefficient this approximation may be adequate, as the amount of flattening of the profile will be negligible if the amount of mass transfer is small in comparison to the mass present in a

given grid block. For dispersion coefficients of the large magnitude possible when enhanced dispersion mechanisms are active, and for the longer time steps desired for numerical dispersion minimization, the concentration gradients may vary significantly over the course of a time step. When small grid blocks and long time steps are used, the dispersive flux across one face of a grid block may be large enough to influence the gradients across the other faces as well, particularly for problems in more than one dimension. Other possible errors may arise in the averaging of the global molar concentrations over two large grid blocks with widely disparate compositions. This could lead to overprediction of the dispersion of components from the block with lower molar density.

The model as described above may be applied directly for two single phase reservoir grid blocks. In the case of multi-phase grid blocks in which the same phases may or may not be present in each block, some rules defining allowable dispersion paths must be used. One option is to allow dispersion based on global mole fractions regardless of the number or type of phases present in each block. A second option is to only allow dispersion within phases that are present in both blocks. Alternatively, Thiebot and Sakthikumar (1991) employ a hypothetical boundary layer consisting of a phase not present in a given grid block; dispersion is allowed into this phase until the absent phase appears in the grid block. The choice of treatment will depend on the type of dispersive forces being modeled. For diffusion alone, the second option or the boundary layer treatment may match the physical process more accurately. When dispersion due to a number of forces is considered, the application of the first option with an appropriate dispersion coefficient may be able to mimic a variety of mixing mechanisms present in the recovery process. For the studies undertaken here, fully miscible fluids are used in all

cases, thus the model formulation as presented initially for two single phase grid blocks is adequate.

As there may be many grid block interfaces with negligible concentration gradients across them, a method of restricting the dispersion calculation to those blocks where it will result in significant effects is desirable. In this model, a minimum change in mole fraction across an interface is specified as an input variable. Each interface is tested at the beginning of the time step, and only those with mole fraction differences exceeding the input minimum are used for the dispersion calculation.

5.1.1. FICK'S FIRST LAW ALGORITHM OUTLINE

To summarize, the steps in the solution of the reservoir flow equations including the first law dispersion model are described below for a two-dimensional system of $i = 1, n_x$ grid blocks in the x direction and $j = 1, n_y$ grid blocks in the y direction.

1. At the beginning of the time step, the pressures, mole fractions and phase properties are all specified and all component dispersive flows are initialized to zero.
2. Do steps 3 through 8 for each $j = 1, n_y$.
3. Do steps 4 through 8 for each $i = 1, n_x - 1$.
4. For each component m with a non-zero dispersion coefficient, the difference in mole fraction across the interface is calculated as

$$\Delta z_m = z_{m,i} - z_{m,i+1} \quad (5.4)$$

5. If the change in mole fraction for any component exceeds the user input value of minimum change for dispersion calculation, go to step 6, if not return to step 3 and increment i .

6. Calculate average global molar density for the grid blocks i and $i + 1$ according to equation (5.1).

7. For each component m the molar flow rate is calculated as

$$q_m = A \phi \rho_{avg} D_m \frac{\Delta z_m}{\Delta x} \quad (5.5)$$

8. These component molar flow rates are added to the component and total molar sources for the grid blocks i and $i + 1$ as:

$$\begin{aligned} q_{m,i} &= q_{m,i} - q_m \\ q_{m,i+1} &= q_{m,i+1} + q_m \\ q_{tot,i} &= q_{tot,i} - q_m \\ q_{tot,i+1} &= q_{tot,i+1} + q_m \end{aligned} \quad (5.6)$$

9. Do steps 4 through 8 again, with $i = 1, n_x$ in the outer loop and $j = 1, n_y - 1$ in the inner loop. Block indices in the above equations are switched from i to j .

10. The convective flow equations and phase behavior equations are solved using the iterative-sequential procedure described in Chapter 3, with the component source rates appearing in equation (3.73) and the overall molar source rates appearing in equation (3.62).

11. Once the pressure equation has converged, the resulting grid block compositions are used to initialize the dispersive flux calculation for the next time step.

5.2. FICK'S SECOND LAW MODEL: LINEAR SEGMENT INITIAL CONDITIONS

This model is developed as an extension of the concepts used in the First law model. Rather than treat each interface individually and assume a constant rate of dispersive flux over the time step, the concentration gradients across each interface are linked to form an approximation to the complete concentration profile. Once this step is

completed, the diffusion equation is solved using the approximate concentration profile as an initial condition and the final shape of the profile can be determined for a change in time equal to the size of the time step. Then for each grid block, the difference between the volumes under the approximate initial profile and the final profile can be used to establish the dispersive flow. For grid blocks of constant cross-sectional area, the difference between the profiles can be established as an area which represents a mole fraction/length product, the volume will then be given by this "area" multiplied by the cross-sectional area. The component molar rate will be equal to the difference between the volumes expressed in moles (by multiplying by the average molar density), divided by the size of the time step. This molar flow rate will then be input explicitly into the convective flow equations as source or sink terms as in the first law model. A schematic diagram showing example initial and final profiles is shown below in Figure 5.2.

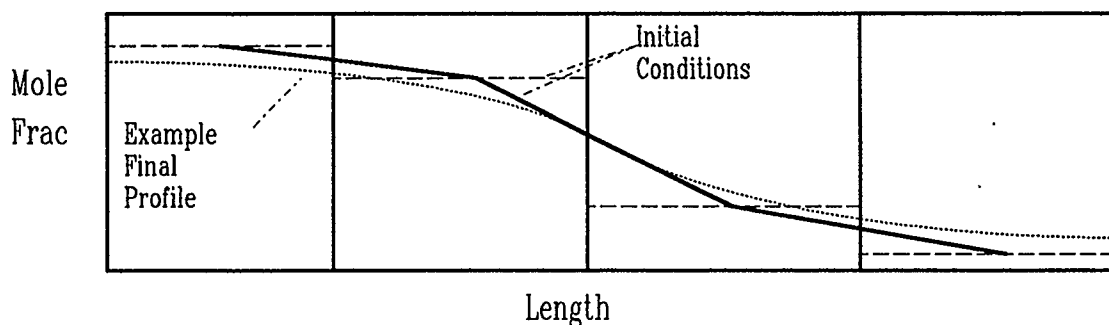


Figure 5.2: Second Law Model Schematic - Approximate Initial Conditions

The initial condition can be approximated in a number of ways. The simplest method is to define the initial condition as a number of horizontal linear segments, equal to the mole fraction of the desired component in each grid block, giving a multiple step function initial condition. Another method is to define gradients as for the First law model, connecting the midpoint of each of the grid blocks and creating a piecewise linear segment initial condition. These two approximations were compared with analytical solutions in section 4.4.3, and were found to match the exact solution profiles with reasonable

accuracy, thus both methods will be investigated here. It should be noted that the piecewise linear segment method will not have the same area under the initial condition curve as the multiple step function method, and it will not contain the same mass of the component as calculated from the convective flow equations. This will not lead to mass balance errors, however, as the dispersive flow rate calculation depends only on the difference between the final and initial profiles, not the absolute magnitudes of the concentrations.

This dispersive flux model will not take into account the simultaneous convective movement and spreading by dispersion of a component profile, rather the amount of dispersive flux will be lagged by one time step behind the convective flux. As for the first law model, the diffusion equation must be solved over a region of constant global molar density. In this case, however, the density must be averaged over all the blocks active in the calculation, not just two blocks. A harmonic average will again be used as follows:

$$\rho_{avg} = \left[\frac{n \prod_{i=1}^n \rho_i}{\sum_{i=1}^n \rho_i} \right]^{1/(n-1)} \quad (5.7)$$

Once this density is calculated, the difference between the areas under the initial and final profiles over the time step may be determined. The area under the initial profile is easily determined. For the multiple step initial condition, the initial area for each grid block is simply equal to the product of the component mole fraction and the grid block length. The area under the final profile for this initial condition will be found from the integration formula given in equation (4.68) for the infinite medium or from equation (4.72) for the bounded medium. The integration formulas are used with x_a and x_b being the locations of the grid block interfaces and t being the length of the time step. For the piecewise linear segment initial condition, the initial area in each grid block is determined from simple

geometric considerations as the sum of two trapezoidal regions. The area under the final profile will be given by the corresponding integration formulas given in equation (4.76) for the infinite medium or in equation (4.80) for the bounded medium. This area is converted into a molar flow rate using the following formula :

$$q_{d,i} = \frac{A \phi \rho_{avg} (A_{initial} - A_{final})}{\Delta t} \quad (5.8)$$

As opposed to the first law model, this molar flow rate already represents the dispersive rate for the block without having to sum the calculated rates for each interface.

As for the first law model, a method of restricting the dispersion calculation to those blocks where it will have significant effects is desirable in the interest of minimizing computing time. Also, since the average molar density over the entire calculation domain must be used for the second law model, the total number of blocks used and their densities will have an effect on the magnitude of the calculated dispersive fluxes. When only one front passes through the reservoir, the selection of the initial and final blocks for the calculation is straightforward. For the initial block, the composition in the first grid block in the row is used as the test composition; this composition is compared to each grid block down the row until a block composition is found to differ by more than some user input tolerance from the test composition. This block will represent the upstream end of the concentration profile and a similar calculation can be done for the downstream side. This calculation is repeated for each component in the system, and the minimum block number obtained for the upstream end is set as the upstream value for all components, similarly, the maximum block number obtained for the downstream end is used for all components.

When more than one front exists in the simulation, the upstream and downstream ends of each profile can be determined and the dispersion calculation will be performed for each profile. The other alternative is to locate the region which encompasses all of the

fronts in the simulation and perform the dispersion calculation for the entire region. This second option is used in this work.

One advantage inherent in the first law method is that mass balance is ensured, as the amount of a component removed from one block is added to the adjoining block. For the second law model, conditions leading to loss of mass balance may be encountered when using the infinite medium forms of the diffusion equation solutions. If the calculation procedure as described above is applied to a complete concentration profile (i.e., one with zero gradients in concentration at each end of the profile) then the dispersive rates calculated for a given component over all of the blocks will sum to zero and mass balance will be maintained. Provided the user input tolerance for locating the ends of the profile is small enough, the calculation will include enough of the profile that any mass balance error will be negligible. When the profile impinges on a boundary of the reservoir, clearly it is impossible to include all of it in the dispersion calculation. Options available for handling this situation include: halting the dispersion calculation, switching the dispersion calculation to the first law model or to the bounded medium form of the diffusion equation solution, or carrying on the dispersion calculation and allowing some degree of mass balance error. These complications could be avoided by employing the bounded medium forms from the start of the simulation, however, these forms include an infinite summation which may require many terms to converge. The severity of the mass balance error and use of these options for limiting it are discussed in Chapter 6.

5.2.1. AUTOMATIC TIME STEP SIZE CONTROL

As discussed in Chapter 3, automatic time step size control is used to maximize the time step size and thus minimize numerical dispersion. For the first law model, the time step size control methods are unaffected, as the dispersion rate is not dependent on the

size of the time steps. In the second law model, however, the rate of dispersion will vary with the time step size. To ensure that negative compositions are not calculated due to the combined dispersive and convective flux of a component being too large, the call to the dispersion subroutine is placed within the automatic time step size control loop at the beginning of a time step. If a negative composition is detected, the time step is reduced and the dispersion calculation is redone to reflect the new time step size.

5.2.2. TWO-DIMENSIONAL DISPERSION MODEL TECHNIQUES

The extension of this model to problems in two dimensions may be accomplished via two approaches. First, the model may be used as described above for each one-dimensional row of grid blocks in the simulation, similar to the approach taken for the first law model. This method has the advantage of simplicity of implementation, both in programming and in derivation of the required integral equations. The second approach would be to define the approximate initial condition in two dimensions, either as horizontal plane segments or as piecewise planar segments. The Green's function method could then be applied to the solution of the diffusion equation with these initial conditions, resulting in equations for the concentration profile which could be then be used to derive two-dimensional forms of the integration formulas. This approach would have the advantage of accounting for dispersive forces in both directions simultaneously. The multiple step initial condition could be easily extended to two dimensions as plane segments equal to the mole fraction in each block, however, the piecewise linear initial condition is not as straightforward to generalize to a piecewise planar condition. For this work, the method of applying the dispersion calculation to a number of one dimensional rows of grid blocks in a two dimensional simulation is described.

5.2.3. FICK'S SECOND LAW ALGORITHM OUTLINE

To summarize, the steps in the solution of the reservoir flow equations including the first law dispersion model are described below for a two-dimensional system of $i = 1, n_x$ grid blocks in the x direction and $j = 1, n_y$ grid blocks in the y direction.

1. At the beginning of the time step, the pressures, mole fractions and phase properties are all specified and all component dispersive flows are initialized to zero.
2. Do steps 3 through 6 for each $j = 1, n_y$.
3. The grid blocks corresponding to the upstream and downstream ends of the profile are located. Each block $i = 1, n_x - 1$ is tested to determine if a component mole fraction in that block differs by more than the user input tolerance from the original upstream fluid composition. When this block is found, the previous upstream block is designated as the upstream end of the profile, denoted by n_1 . The composition test is continued to locate the block corresponding to the downstream end of the profile where the component mole fraction differs less than the input tolerance from the original downstream fluid composition. This block is denoted n_2 .
4. The average global molar density for grid blocks n_1 through n_2 is calculated according to equation (5.7).
5. For each block, $i = n_1 \dots n_2$, and for each component m , the initial area is calculated. For the multiple step initial condition the initial area is given by

$$A_{initial} = z_{m,i} \Delta x \quad (5.9)$$

For the piecewise linear initial condition the initial area is given by

$$A_{initial} = \frac{\Delta x}{8} (z_{m,i-1} + 6z_{m,i} + z_{m,i+1}) \quad (5.10)$$

The final areas are calculated from equation (4.68) for the infinite medium multiple step function, equation (4.72) for the bounded medium multiple step function, equation (4.76) for the infinite medium piecewise linear function, and equation (4.80) for the bounded medium piecewise linear function.

6. The molar flow rate corresponding to the change in area is calculated from equation (5.8) for each component, and the total dispersive flow rate for the grid block is summed over all components.

7. Do steps 3 through 6 again, for $i = 1, n_x$. Block indices in the above equations are switched from i to j .

8. The convective flow equations and phase behavior equations are solved using the iterative-sequential procedure described in Chapter 3, with the component source rates appearing in equation (3.73) and the overall molar source rates appearing in equation (3.62).

9. Once the pressure equation has converged, the resulting grid block compositions are used to initialize the dispersive flux calculation for the next time step.

5.3. FICK'S SECOND LAW MODEL: FRONT TRACKING ALGORITHM

This model is developed in an attempt to describe dispersive processes which may take place on a scale smaller than one grid block. Solutions of the diffusion equation are again employed, however the initial conditions are determined not as gradients across a number of grid blocks, but rather as step functions at injection points or at significant compositional discontinuities within the reservoir. The dispersion profile resulting from the solution of the diffusion equation with the step function initial condition is then superimposed on top of the convective movement of the front, assuming a piston-like convective flow. The inclusion of dispersive fluxes in the source terms of the convective

flow equation as for the previous two models is employed only when a significant portion of the profile is intersecting a grid block interface. As shown in the schematic below in Figure 5.3, no dispersive flux across the interfaces will be taking place in the example at left, while dispersive flux across three interfaces will be occurring in the example profile on the right.

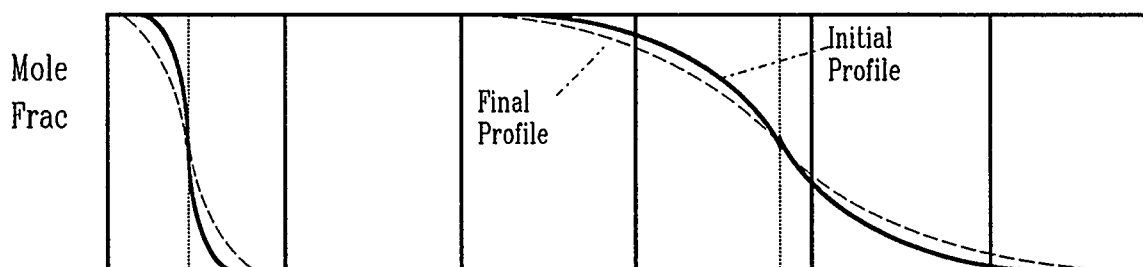


Figure 5.3: Second Law Model Schematic - Front Tracking Algorithm

As for the previous model, the amount of dispersive flux over a time step is determined as the difference between the areas under the profile at the beginning and end of the time step. For the case of a constant dispersion coefficient, the profiles are calculated from the solution of the diffusion equation for a step initial condition given in equation (4.52) for the infinite medium, with the corresponding areas under the curve given by the integration formula given in equation (4.57). The corresponding formulas for the bounded medium are given in equation (4.59) and (4.61). The area under the initial profile is calculated by applying equation (4.57) or (4.61) with time being entered as the total elapsed time from the initiation of the step initial condition to the beginning of the time step. The area under the curve at the end of the time step is calculated using the same formula with time entered as the total elapsed time to the end of the time step. If a variable dispersion coefficient is employed, the shape of the profile may be calculated from the step initial condition up until the time at which the dispersion coefficient is to be changed. At this point, the profile is divided into an arbitrary number of segments and is approximated using one of the linear approximations discussed in the previous section. Once this shape

is approximated, the areas under the curve at the beginning and end of a time step may be determined as for the previous model. The use of a constant global molar density is again required for solution of the diffusion equation; the harmonic average as discussed above is used in this model as well.

As for the second law model, the front tracking algorithm lags the dispersion calculation one time step behind the convective flow calculation. In this model the interface compositions which multiply the transmissibility terms in the convective flow equations are modified to reflect the shape and location of the dispersion profile, this transmissibility modification is also lagged by one time step behind the convective flow calculation. In the standard single-point upstream weighting scheme, the interface compositions are set equal to the block average compositions. In the front tracking model, a component's interface composition will be set according to the value of the composition profile at that interface. If the profile does not cross the interface, the interface composition will be set to zero, regardless of the average composition in the grid block. If the profile does cross an interface, the interface composition is calculated as follows: the amount of bulk movement of the profile through convective transport which occurred in the last time step is calculated from the pressure gradient and transmissibility values at the end of the time step. The portion of the profile which moved past the interface due to the bulk convective flow is then integrated to determine the number of moles of the component which were transferred across the interface. Finally, the constant mole fraction required to produce this same molar transport is calculated and used as the interface composition.

To initialize the calculation, the user must input the number of fronts, their locations and the initial upstream and downstream compositions for each front. For a front

located at an injection point, the distance traveled by the piston-like convective front in one time step is calculated as:

$$\Delta x_f = \frac{Q\Delta t}{A\phi} \quad (5.11)$$

when the front is in the block containing the injector. When the front has traveled out of the first block into any grid block i , or for any other front which was not originally located at an injection point, this distance is calculated as:

$$\Delta x_f = \frac{T_{x,i-1}(P_{i-1} - P_i)\Delta t}{A\phi\rho_{i-1}} \quad (5.12)$$

The "active" interfaces, those which will have dispersive flux across them, are located by first locating the midpoint of the convective front. This is the distance that the initial step condition will have traveled due to the assumed piston-like convective flux. To locate the downstream end of the profile, the value of concentration at each interface in front of the profile midpoint is calculated for the total elapsed time since the step initiation. When an interface is reached which has a calculated concentration less than some user input tolerance, that point is taken to be the downstream end of the profile. Similarly for the upstream end, when an interface is located which has a component concentration different by less than the tolerance from the original upstream composition, that is taken as the upstream end of the profile.

Once the active interfaces are located, the change in area calculation is carried out to determine the amount of dispersive flux. This calculation is implemented in the same way as for the previous model, with the difference in areas being converted into molar rates using equation (5.8). Again, use of the integration method for determining these fluxes can lead to the propagation of mass balance errors. When a profile is located wholly within the reservoir domain, mass balance can be assured by performing the integrations

within a symmetrical region encompassing equal distances in front of and behind the front midpoint. Thus, depending on the location of the midpoint, the integration in either the first or last grid block will be restricted to a length less than the total length of the block. When the profile impinges on a reservoir boundary, a symmetrical region must still be used, with the length of the region being dictated by the distance the front midpoint is from the reservoir boundary. This will result in the dispersion calculation for the trailing edge of the profile being terminated prematurely. In this case, the dispersion calculation could revert to the first law model for the remainder of the calculation. As the magnitude of the inter-block dispersion in this model does not depend on the size of the current time step, the automatic time step size control as outlined in Chapter 3 can be used without modification.

5.3.1. SECOND LAW MODEL: FRONT TRACKING ALGORITHM OUTLINE

The steps in the front tracking algorithm for a one-dimensional system with grid blocks $i = 1, n_x$, grid block length Δx , and a constant dispersion coefficient are given below for a single front application. The steps in the calculation may be repeated for as many fronts as required.

1. At the end of the time step, the pressures, mole fractions and phase properties are all specified and all component dispersive flows are initialized to zero.
2. The distance that the midpoint of the front has moved during this time step is calculated from equation (5.11) or (5.12). The location of the front x_f is calculated as the sum of these steps, and the grid block that the front falls in is designated as n_f .
3. The grid blocks corresponding to the upstream and downstream ends of the profile for each component are located. The downstream end is located by setting $n = n_f \dots n_x$ and calculating the distance from the profile midpoint to the block n interface from

$$x = n\Delta x - x_f$$

(5.13)

This value is input as the x -variable in equation (4.52) with a time value equal to the elapsed time from the step function initiation to determine the component concentration at that interface. If the concentration is less than the user specified tolerance, that grid block is designated the downstream end of the profile, n_2 . For the upstream end, the block indicator is varied from $n = n_f \dots 1$ and equation (5.13) is again used to generate the x -variable. In this case, when the calculated concentration differs by less than the tolerance from the original composition, that block is designated as the upstream end of the profile, n_1 .

4. The average global molar density for grid blocks n_1 through n_2 is calculated according to equation (5.7).

5. For each block, $i = n_1 \dots n_2$, and for each component m , the initial area is calculated from the integration formula given in equation (4.57), with x_a and x_b input as the block interface locations and time input as the elapsed time to the start of the time step. The final area is calculated in the same way with the time input as the elapsed time to the end of the time step. The change in areas is converted into a molar rate using equation (5.8), and is designated $q_{m,n}$ for component m and grid indicator n .

6. For each block, the molar flow rates are summed over all components to give the total molar rate for that block.

7. For all blocks excluding n_1 through n_2 , the interface compositions are set using the standard single-point upstream weighting scheme. For each interface active in the dispersion calculation, the interface composition is set by integrating the portion of the profile which will cross the interface in the next time step. For grid blocks $n = n_1 \dots n_2$, the integration formula given in equation (4.80) is used to evaluate the area A under the curve between the points

$$\begin{aligned}x_b &= n\Delta x - x_f \\x_a &= x_b - \Delta x_f\end{aligned}\tag{5.14}$$

The interface composition is then given by

$$z_{m,i} = A/\Delta x_f\tag{5.15}$$

8. The convective flow equations and phase behavior equations are solved using the iterative-sequential procedure described in Chapter 3, with the component source rates appearing in equation (3.73) and the overall molar source rates appearing in equation (3.62).

9. Once the pressure equation has converged, the resulting grid block compositions are used to initialize the dispersive flux calculation for the next time step.

5.4. SUMMARY

Algorithms for incorporating Fick's first law and solutions of Fick's second law have been described in this Chapter for treatment of dispersion in a compositional reservoir simulator. The first law models are readily applicable to multi-dimensional problems. One simple approach for two-dimensional simulation employing the second law models based on solution of approximate initial conditions has also been described. The front tracking algorithm was developed for use in only one dimension. These models are tested for three example model geometries in the following Chapter.

6. APPLICATION OF COMPOSITIONAL SIMULATOR WITH DISPERSION MODELS

The models developed in the previous chapter are used here for the simulation of the Taylor dispersion experiment as discussed in Chapter 2, the visual experiment introduced in Chapter 1 and a typical laboratory slim tube test. The general compositional reservoir simulator described in Chapter 3 and the dispersion models described in Chapter 5 have been coded in FORTRAN to run on the University of Calgary's network of AIX workstations with RISC 6000 architecture. Running on the network sometimes precludes the direct comparison of computing times as jobs can be run on platforms with different characteristics; for example the rs6000.950 file server can perform a job roughly 3 times faster than the rs6000.220 workstation. When run times are compared, an approximate correction will be applied to normalize the times to a single machine type.

6.1. TAYLOR DISPERSION EXPERIMENT SIMULATION

The first system studied is the experimental Taylor dispersion apparatus simulated with the conventional compositional model in Chapter 2. Ethane will be used as the solvent for all runs, and the oil slug will be modeled as n-octane or the 5 component reservoir oil model as described in Table 2.1. As described in Chapter 2, the apparatus is used to investigate dispersion at the leading and trailing edges of an oil slug within a stream of solvent as the slug is transported through a length of capillary tubing. A constant injection rate of solvent is specified at one end of the tube and a constant back pressure constraint equal to the initial pressure in the tube is specified at the production end. The physical parameters used in the simulation are shown in the following table.

Table 6.1: Parameters for Taylor Dispersion Experiment Simulation

Length	$x = 8.607 \text{ m}$
Solvent Zone 1	$0 < x < 1.208 \text{ m}$
Oil Slug Zone	$1.208 < x < 2.416 \text{ m}$
Solvent Zone 2	$2.416 < x < 8.607 \text{ m}$
Height and Width	$\Delta y = \Delta z = 0.07071 \text{ cm}$
Porosity	100%
Permeability	$2.0 \times 10^4 \text{ darcy}$
Pressure	22.75 MPa
Temperature	372.05 K
Solvent Injection Rate	0.2 mL/hr

6.1.1. FIRST LAW DISPERSION MODEL

Clearly, to gauge the effects of the physical dispersion models accurately, the amount of numerical dispersion present for a given system must be quantified, and hopefully minimized. To provide a basis for the study, several runs of the simulator using the first law dispersion model were performed for the ethane + n-octane system with one point upstream weighting of the compositions, that is, with no numerical dispersion control. In this case, the amount of numerical dispersion can be minimized only by using a fine grid and the maximum stable time step size, as discussed in section 3.2.9. The maximum time step size is determined by the throughput stability criterion which requires that no more than one grid block pore volume of material be passed through a block in one time step. As discussed in Chapters 3 and 5, automatic time step control is used within the simulator to check that this condition is not being violated.

A fine grid model consisting of 912 grid blocks was used for these initial runs. This corresponds to 128 grid blocks for the original oil slug. The simulation is run for 80,000 s and process variables are output every 500 s. The maximum allowable change in mole fraction over a time step is set to 0.8 so that the time step sizes will not be limited by this factor. A rough limit to the maximum time step size may be determined from the injection

rate and the pore volume of a single grid block; this yields a value of 85 s to be input as the maximum time step size. When the dispersion calculation is active, however, the combined dispersive and convective fluxes will most likely require that the simulator reduce the time steps below this level.

Using these parameters, simulations were performed with $D = 0$, 10^{-3} , and 10^{-2} cm²/s. The same value of dispersion coefficient was used for each component in the system. The minimum change in mole fraction used to limit the dispersion calculation is set at 10^{-8} ; this allows the calculation to be carried out well into the trailing edges of the profile and thus will not prematurely cut off the ends of the profile. The results of the simulations were found to be insensitive to the mole fraction cutoff for tests of the value between 10^{-2} and 10^{-8} . To give an indication of the level of dispersion which could be expected with the above coefficient values, profiles were calculated with the standard error function solution to the step initial condition. With $D = 0$, of course, the solution is simply the initial step conditions translated to account for the amount of fluid injection. For the non-zero coefficients the profile reflects the sum of the solutions for the two step initial conditions. The simulated results will differ from these profiles since the error function solutions do not take into account the shrinkage which will be occurring on mixing of the solvent and oil; however the comparison is instructive for observing the magnitude of the differences in the analytical profiles calculated with different dispersion coefficients. The results of these calculations are shown in Figure 6.1. The effluent mole fraction of the oil model component is plotted versus the volume of solvent injected expressed in reservoir cm³, that is at the pressure and temperature of the block containing the injector.

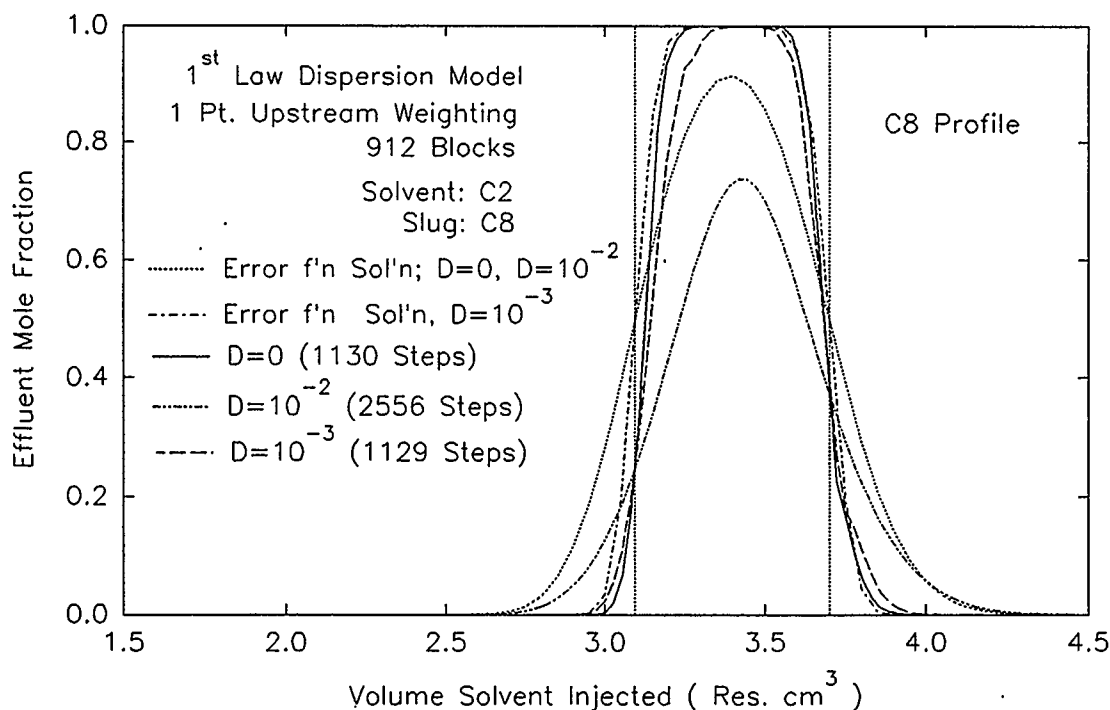


Figure 6.1: Taylor Experiment Simulation, Ethane + n-Octane, First Law Dispersion Model with Single Point Weighting

The simulated results obtained with $D=0$ show fair agreement with the error function solution in terms of location and integrity of the slug, however the edges of the slug are smeared to some degree through numerical dispersion. This simulated profile actually appears to compare quite closely with the error function solution with a dispersion coefficient of $D=10^{-3}$ cm²/s. The simulated results obtained with $D=10^{-3}$ cm²/s show some effect of the physical dispersion in addition to that associated with the numerical dispersion. The amount of numerical dispersion for both the $D=0$ and $D=10^{-3}$ cm²/s runs will be the same as both required the same number of time steps (1130) to complete the run. The simulation for $D=10^{-2}$ cm²/s required more than double this number of time steps (2556) as the higher level of dispersive flux forced the simulator to reduce the time step size to avoid transferring more moles of a component out of a block during a time step than existed at the start of the time step. In this case non-convergence of the pressure

equation also caused the simulator to reduce the time step size in some instances, as the large number of blocks and the high dispersive fluxes make the solution of the equation more difficult. This large number of steps means that the level of numerical dispersion for this case will be higher than for the other two simulated results discussed above.

In comparison to the error function profile, the leading and trailing edges of the simulated profile are located correctly. With the obviously large negative volume change occurring due to the high degree of mixing, as indicated by the difference in the areas under the profiles, it is impossible to determine if the correct amount of mixing has been predicted, and to what extent the numerical dispersion has influenced the final shape of this profile.

The run times for these simulations were on the order of 30 minutes for the $D = 0$ and $D = 10^{-3} \text{ cm}^2/\text{s}$ runs and approximately 70 minutes for the $D = 10^{-2} \text{ cm}^2/\text{s}$ run on the

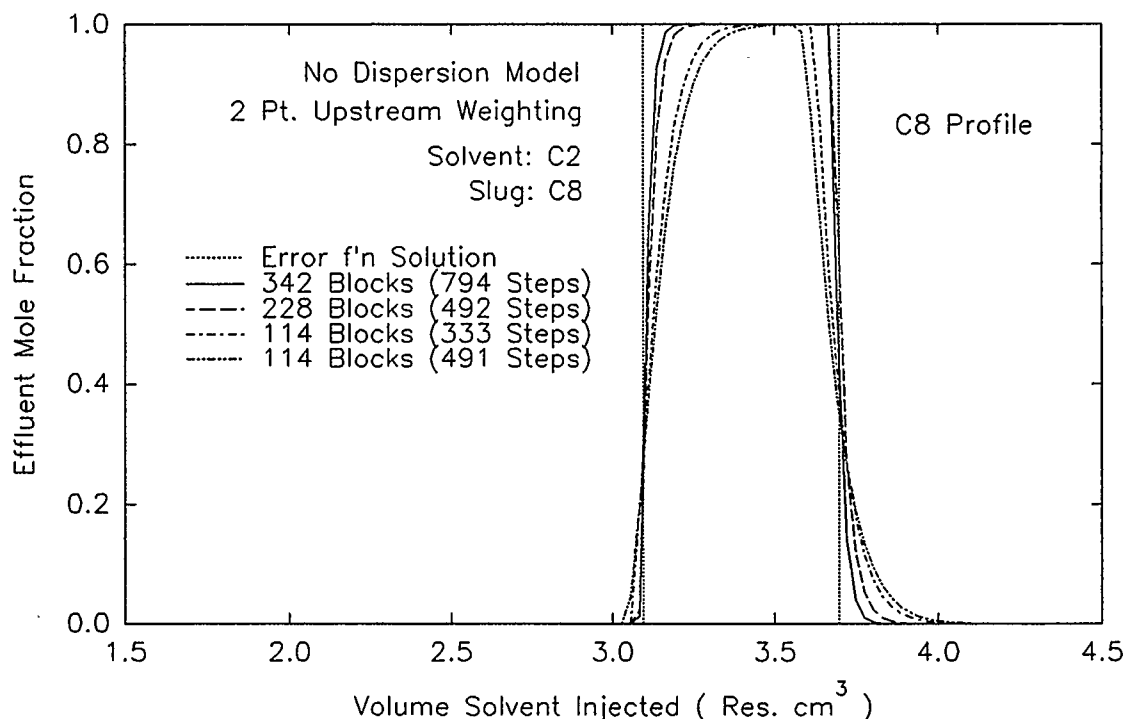


Figure 6.2: Taylor Experiment Simulation, Ethane + n-Octane, No Dispersion Model with Two Point Weighting

rs6000.950 platform.

In the interest of reducing run times, and also to allow running with roughly equal numbers of time steps whether high levels of physical dispersion are introduced or not, the two point upstream weighting in composition was investigated next. Simulated results with $D = 0$ for model systems of 114, 228 and 342 grid blocks, corresponding to the oil slug containing 16, 32, and 48 grid blocks respectively, are shown in Figure 6.2. Again the error function solution with $D = 0$ representing the width of the original oil slug is shown for comparison. Time step size controls were set again to allow the simulator to select the largest possible step sizes to minimize numerical dispersion, subject to the restriction of obtaining data at 500 s increments. The runs with 342 and 228 grid blocks show less numerical dispersion than the single point upstream weighting run with 912 grid blocks. Two runs were performed for the 114 grid block case: one with the simulator selecting the optimal time step size resulting in 333 time steps for completion, and one with the step length restricted, resulting in a run of 492 time steps. This was done to observe the relative change in numerical dispersion incurred for this system with a constant number of blocks but with a varying number of steps to completion. Increasing the number of steps by approximately 50% in this case is seen to have a noticeable, but not excessive, effect on the amount of numerical dispersion.

All of the calculated profiles show an asymmetry introduced by the two point weighting technique, with the leading edge of a front being truncated more strongly than the trailing edge. This is a numerical artifact and does not reflect a physical asymmetry in the profile. However, this disadvantage of two-point weighting is outweighed by the ability to perform runs with a relatively small number of grid blocks and still have minimal numerical dispersion. The run times for these simulations ranged from 1.5 min for the 114 grid block case to 13 min for the 342 grid block model on an rs6000.340 workstation; this

machine is roughly 25% slower than the rs6000.950 for which the single point model run times were reported. The remainder of the first law dispersion model test runs are performed with the two-point upstream weighting technique.

Simulations were performed using the configurations discussed above for $D = 10^{-2} \text{ cm}^2/\text{s}$ and $D = 10^{-3} \text{ cm}^2/\text{s}$. The results are shown in Figures 6.3 and 6.4 respectively. Again, the error function profiles are shown for comparison. For the $D = 10^{-2} \text{ cm}^2/\text{s}$ case, the simulated profiles obtained with 228 and 342 grid blocks very nearly coincide, and the 114 grid block case with maximum time steps allowed actually shows less total dispersion than the others. When the 114 grid block model is used with restricted time steps is used, the amount of dispersion is increased and a much higher volume change on mixing effect is observed. This is the result of the combination of large blocks and the dispersion model creating contact between larger volumes of oil and solvent than will be occurring with the finer grid models. Increasing the amount of numerical dispersion by restricting the time steps amplifies the effect.

All of the profiles show more truncation of the leading edge of the profile than the trailing edge, illustrating that the two point upstream weighting will reduce not only numerical dispersion, but also the physical dispersion effects.

For the runs with $D = 10^{-3} \text{ cm}^2/\text{s}$, the incremental dispersion added by the physical dispersion model is nearly reduced to zero by the two point weighting. All of the curves are almost identical to those obtained with $D = 0$ and the volume change effects seen for the previous case are not a factor. In this case, the total amount of dispersion is more a function of the number of grid blocks in the simulation than it is of the physical dispersion model.

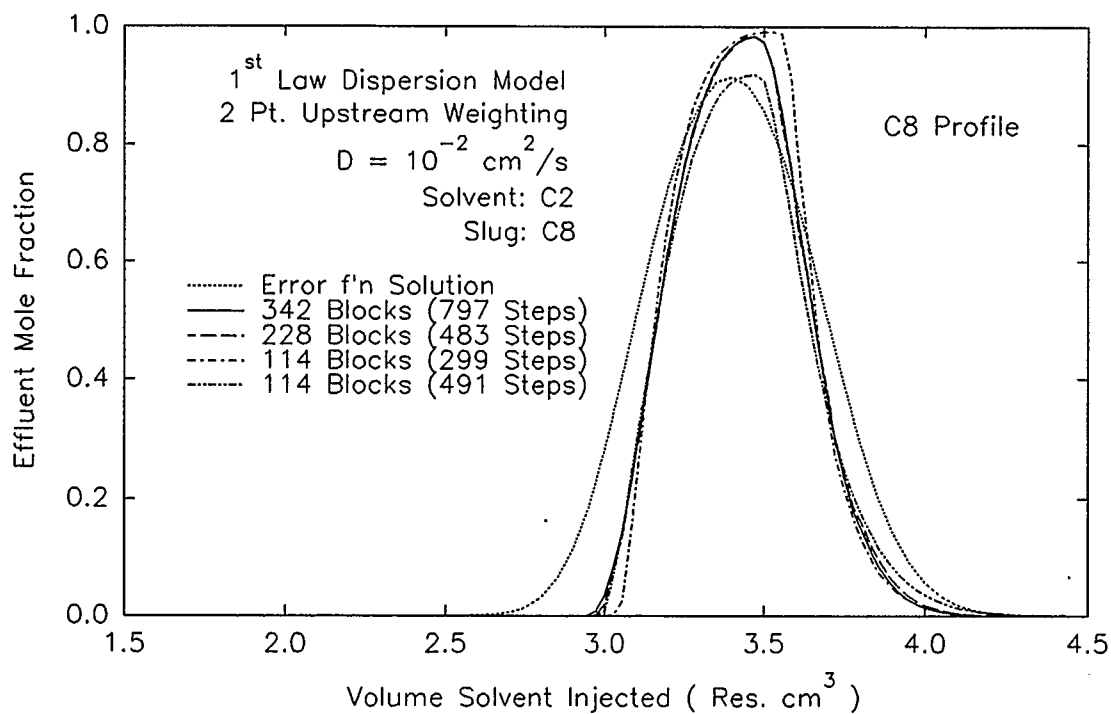


Figure 6.3: Taylor Experiment Simulation, Ethane + n-Octane, First Law Model with $D = 10^{-2} \text{ cm}^2/\text{s}$

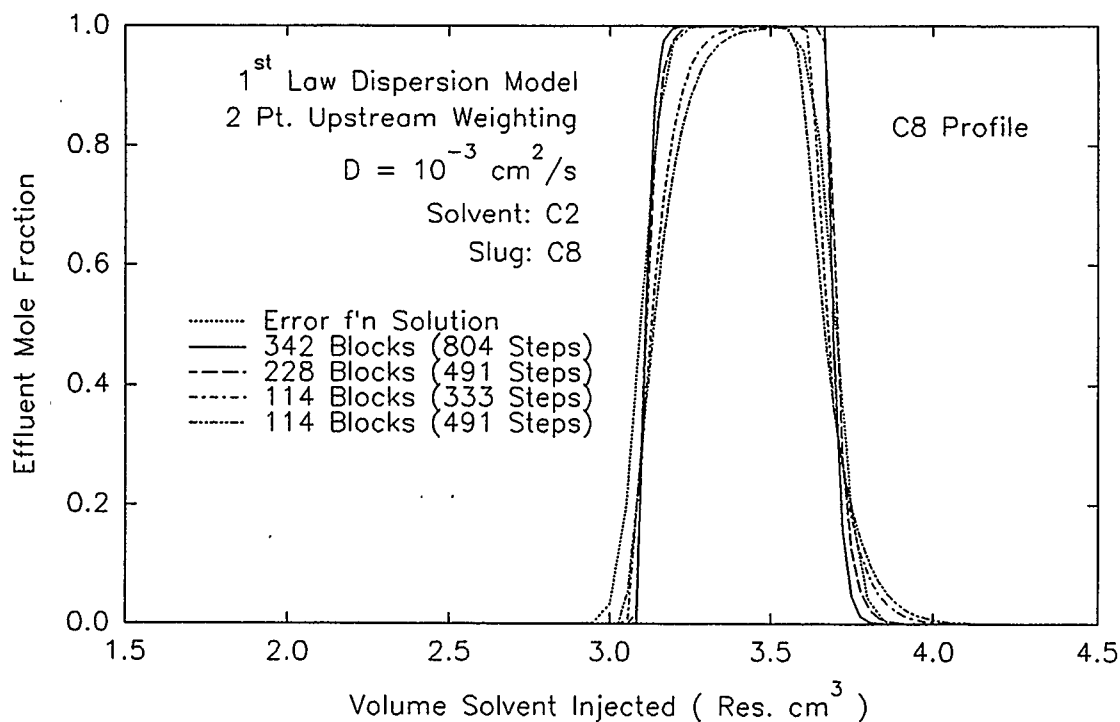


Figure 6.4: Taylor Experiment Simulation, Ethane + n-Octane, First Law Model with $D = 10^{-3} \text{ cm}^2/\text{s}$

Next, the first law model is applied to the case of ethane solvent contacting the 5 component reservoir oil model, using the same grid block configurations as for the ethane + n-octane runs. Again, the simulations were performed first with $D = 0$ to determine how the simulator performed on the multicomponent system. The results of these runs are shown in Figure 6.5. The run times on the rs6000.340 range from 3 min for the 114 grid block case to 17 min for the 342 grid block case. The same trends observed in the ethane + n-octane runs are observed here.

The results for the ethane + 5 component oil with $D = 10^{-2} \text{ cm}^2/\text{s}$ are shown in Figure 6.6. The number of time steps required for these runs are comparable to (although slightly less than) those required when no dispersion coefficient was used, resulting in run times of 2 min for the 114 grid block case and 13 min for the 342 grid block case. As for the ethane + n-octane runs, the profiles generated from the 228 and 342 grid block runs

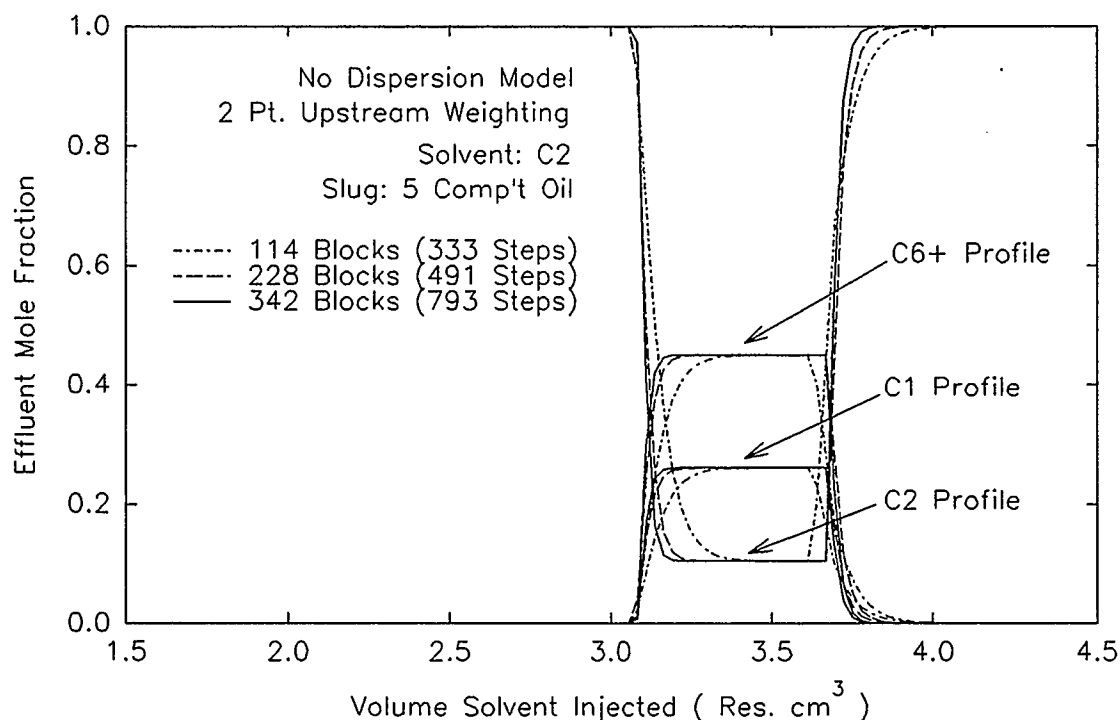


Figure 6.5: Taylor Experiment Simulation, Ethane + 5 Component Oil, No Dispersion Model with Two Point Weighting

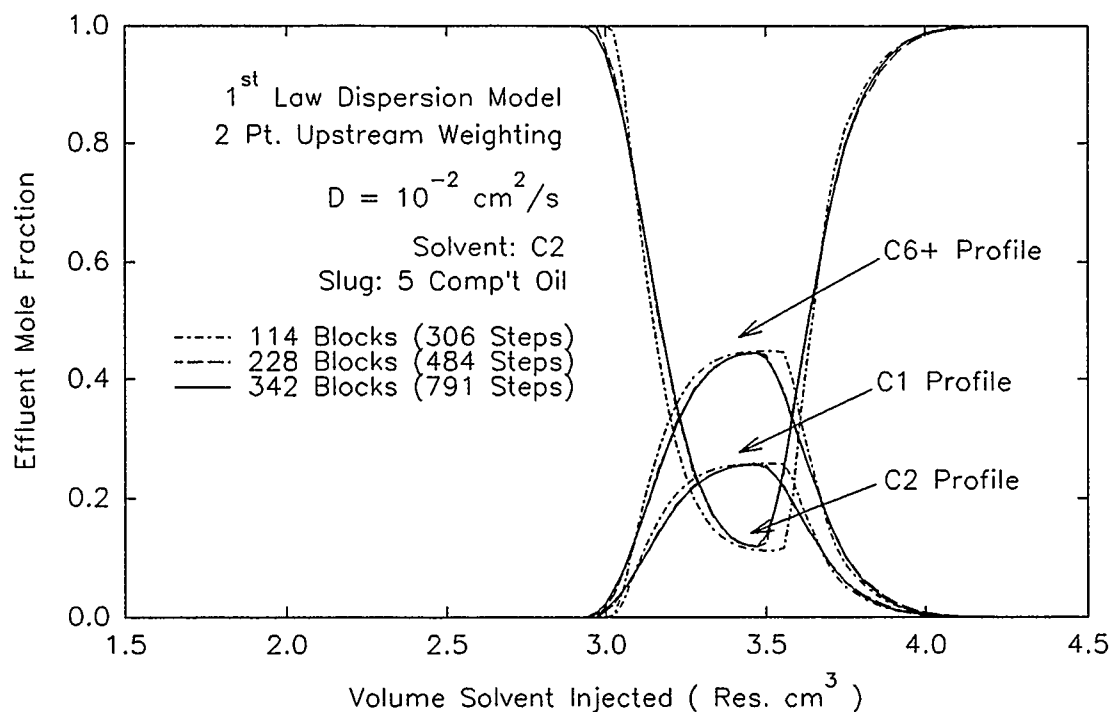


Figure 6.6: Taylor Experiment Simulation, Ethane + 5 Component Oil, First Law Dispersion Model with $D = 10^{-2} \text{ cm}^2/\text{s}$

are nearly identical, and the 114 grid block run shows less total dispersion than the others. In comparison to the experimental results for this system presented in Chapter 2, the width of the dispersed zone is predicted reasonably well by the first law model, although the leading edge of the profile is again truncated by the two point weighting technique. The component mole fraction peaks predicted by the model differ significantly from the experimental ones, however this is due at least in part to the 5 component oil characterization.

It is also noted that the non-physical inflections in the profile obtained with the EOSIM simulator are not seen in the profiles calculated with the model developed for this work. The EOSIM model uses two-point weighting on relative permeabilities and other phase properties as well as composition, and applies filtering mechanisms which can create these types of inflections when used for systems which exhibit significant volume change

on mixing. The simplicity of the two-point upstream weighting on composition used in the present work is apparently not susceptible to this problem.

These results indicate that, for the Taylor dispersion experiment, the first law method can model the profiles obtained when a significant degree of physical dispersion is present in the system. Two-point upstream weighting techniques are valuable for reducing the amount of numerical dispersion in a system, however they also reduce physical dispersion when it is present. When smaller values of the dispersion coefficient are used, the numerical dispersion control technique nearly reduces the amount of physical dispersion to zero.

6.1.2. SECOND LAW DISPERSION MODEL: APPROXIMATE INITIAL CONDITIONS

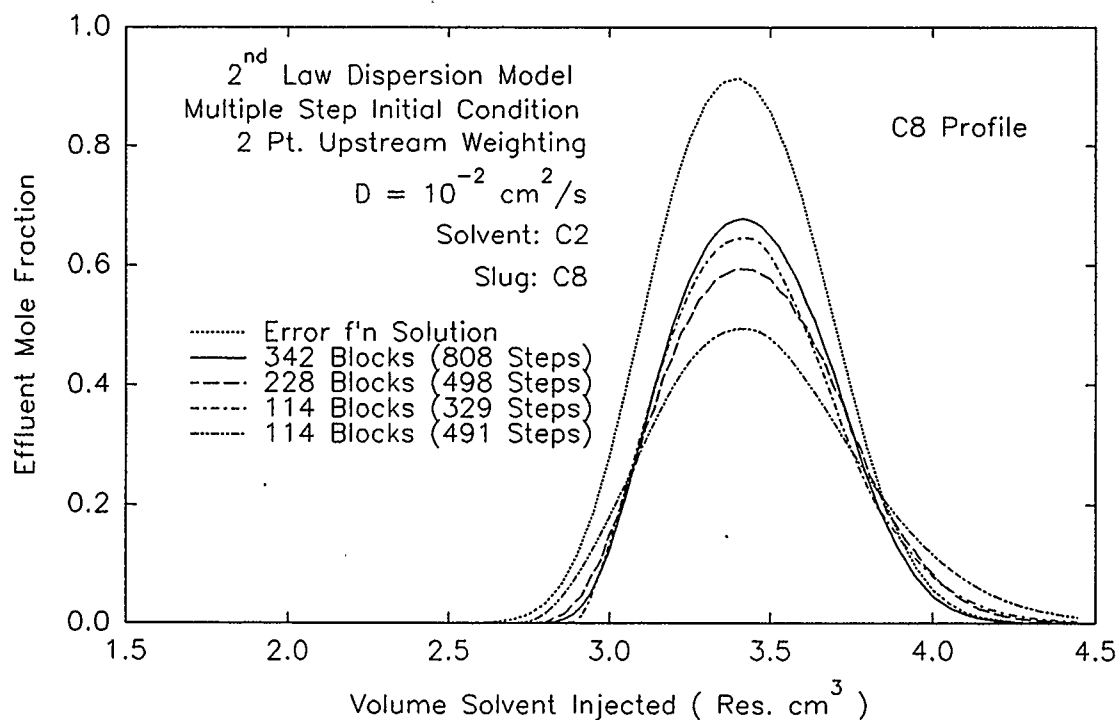


Figure 6.7: Taylor Experiment Simulation, Ethane + n-Octane, Second Law Multiple Step Dispersion Model with $D = 10^{-2} \text{ cm}^2/\text{s}$

The second law dispersion model is tested initially for the ethane + n-octane system using the two point upstream weighting and grid block configurations as for the first law model. The mole fraction tolerance for locating the initial and final blocks of the profile is again set to 10^{-8} and a single region is used for the dispersion calculation, that is, the calculation is performed for a region encompassing the leading and trailing edges of the slug, rather than performing a separate calculation for each edge. The first runs are performed using the multiple step initial condition with $D = 10^{-2} \text{ cm}^2/\text{s}$; the results are shown in Figure 6.7.

The model is over-predicting the amount of dispersion in this case, in comparison to both the error function solution and the results shown previously for the first law model. The high degree of mixing predicted leads to large volume changes, resulting in the decreasing size of the profiles in the figure. The multiple step solution to the diffusion

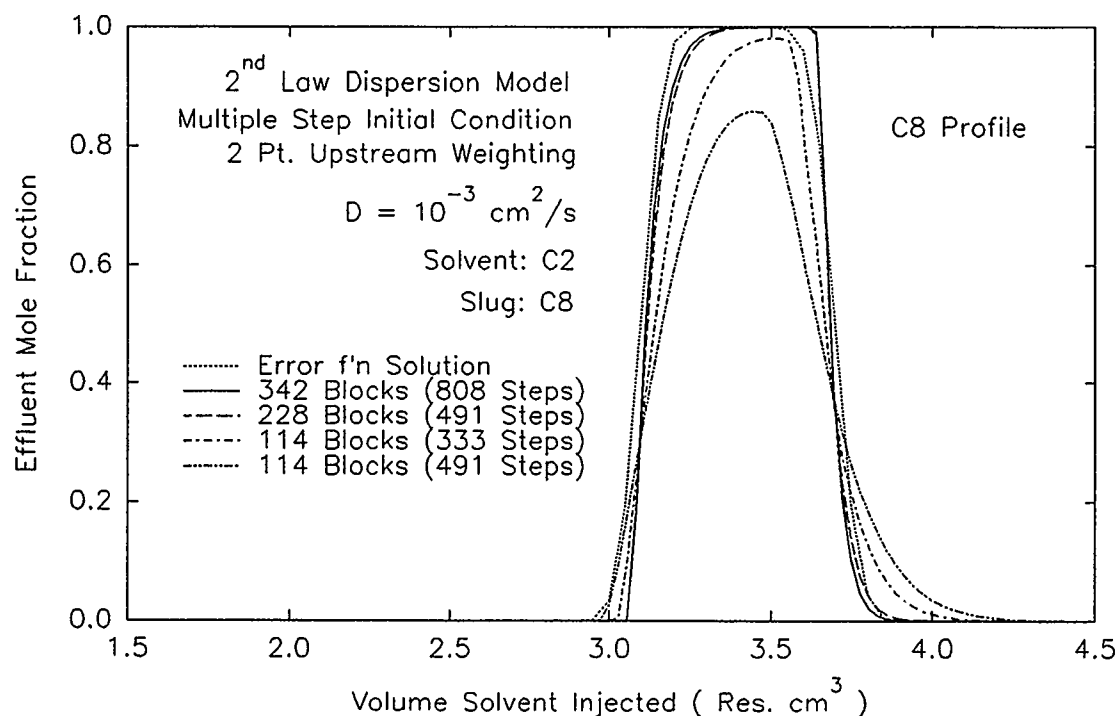


Figure 6.8: Taylor Experiment Simulation, Ethane + n-Octane, Second Law Multiple Step Dispersion Model with $D = 10^{-3} \text{ cm}^2/\text{s}$

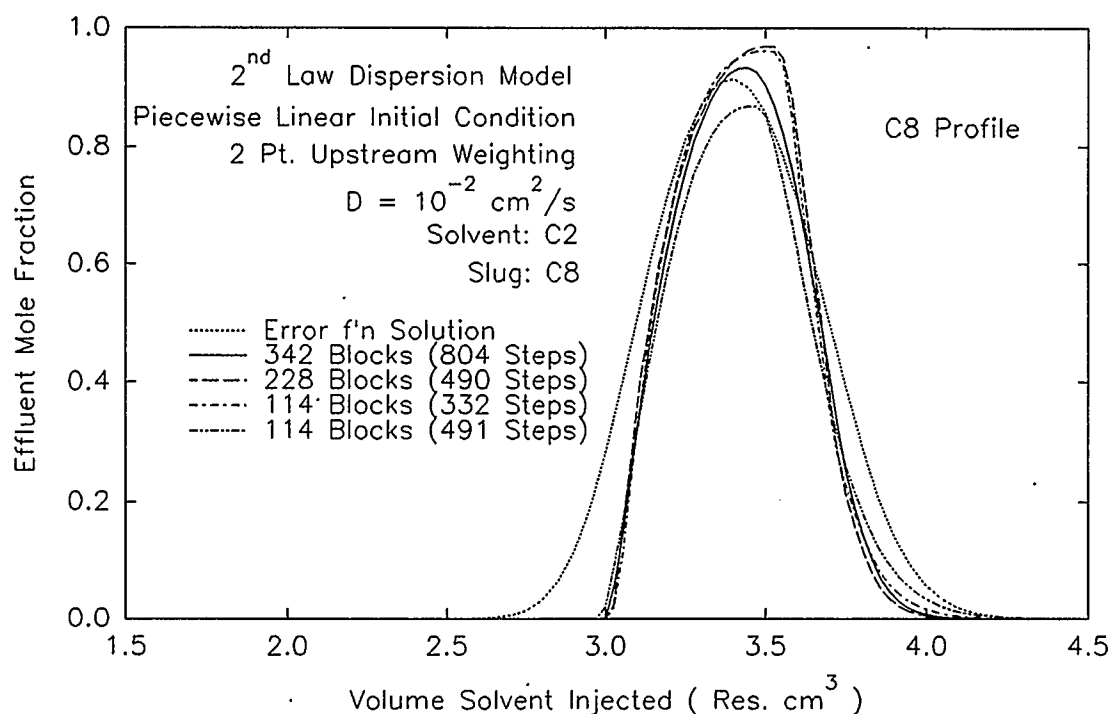


Figure 6.9: Taylor Experiment Simulation, Ethane + n-Octane, Second Law Piecewise Linear Dispersion Model with $D = 10^{-2} \text{ cm}^2/\text{s}$

equation was shown in Chapter 4 to be adequate for several time small time steps. In the application here, however, the size of the time steps is large enough that over the course of the simulation the degree of dispersion is greatly exaggerated. The results obtained from this model for $D = 10^{-3} \text{ cm}^2/\text{s}$ are shown in Figure 6.8. Although the effects are not as significant in this case, overprediction of the dispersion is still occurring.

These runs were repeated with the same configuration but using the piecewise linear initial condition approximation. The results obtained with $D = 10^{-2} \text{ cm}^2/\text{s}$ are shown in Figure 6.9. The profiles obtained in this case are much more similar to the error function solution and the results from the first law model than those resulting from the multiple step approximation. As opposed to the first law results, however, the results for the 114 and 228 grid block cases are quite similar in this case, while the 342 grid block case shows more dispersion; again, the amount of volume change on mixing for the 114 grid block

case is strongly dependent on the number of time steps taken. As the number of time steps taken for both the first law and second law models are similar, differences in the profiles are due to the physical dispersion models.

As discussed in Chapter 5, mass balance errors can occur when using the profile integration method of determining dispersive flux. The mass balance check procedures introduced in Chapter 3 are used over each time step, and over the course of the entire simulation to ensure mass is not being created or lost. The overall mass balance check gives a ratio of initial moles plus injected moles over final moles plus produced moles for each component. For these runs of the second law model, the profile was simply truncated at the point where it impinged on the reservoir boundary. The worst mass balance ratio for these runs was 0.99496, roughly 0.5%, calculated for n-octane in the 114 grid block case. As this amount of mass balance discrepancy will not manifest itself as a significant error in

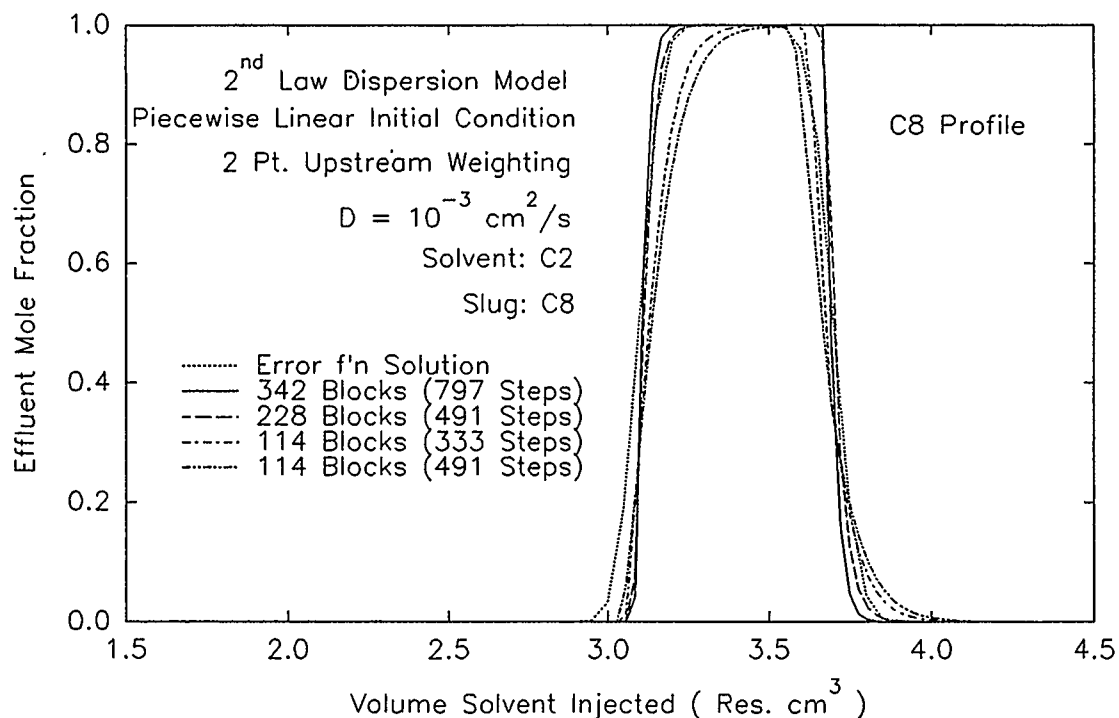


Figure 6.10: Taylor Experiment Simulation, Ethane + n-Octane, Second Law Piecewise Linear Dispersion Model with $D = 10^{-3} \text{ cm}^2/\text{s}$

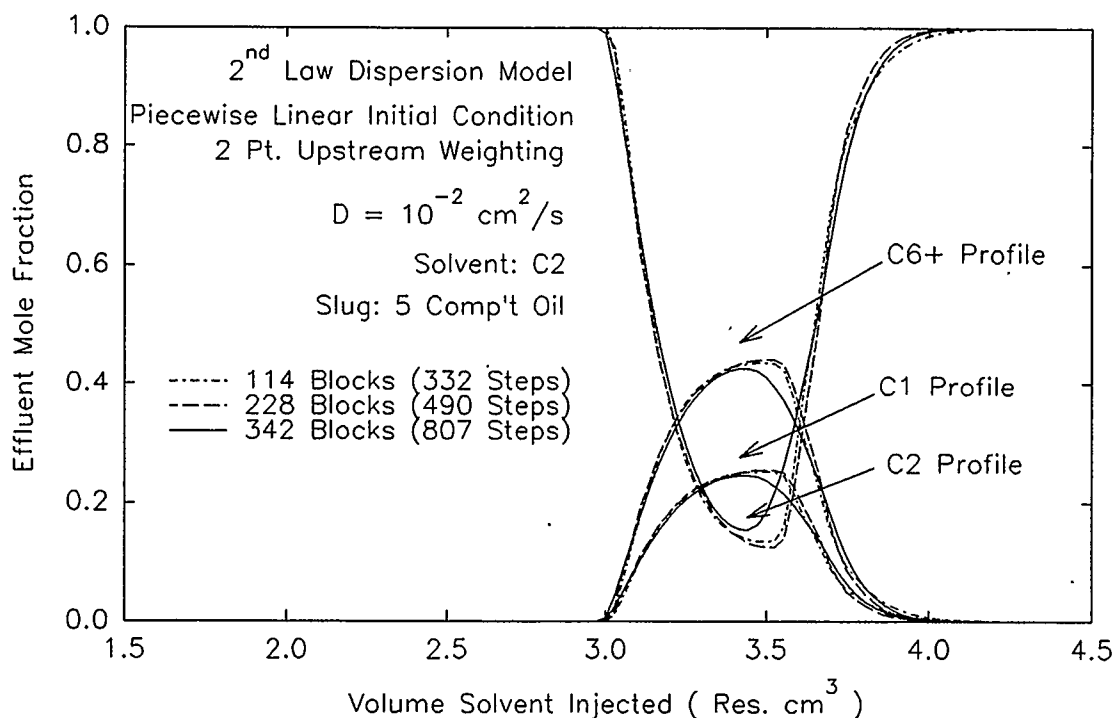


Figure 6.11: Taylor Experiment Simulation, Ethane + 5 Component Oil, Second Law Piecewise Linear Dispersion Model with $D = 10^{-2} \text{ cm}^2/\text{s}$

terms of the effluent mole fractions and other process variables, no action in terms of modifying the calculation was undertaken. The mass balance ratio was monitored for all runs to make sure that this situation did not change.

The results obtained for the piecewise linear approximation model with $D = 10^{-3} \text{ cm}^2/\text{s}$ are shown in Figure 6.10. In this case the calculated profiles for all configurations are indistinguishable from those calculated with the first law model. This result shows that the gradients calculated for the first law dispersion model remain nearly constant over a time step, thus the mass transfer calculated by integrating the profiles corresponds exactly to that calculated from the constant interfacial gradient assumption.

Finally, this model is applied to the ethane + 5 component oil model; the results are shown in Figure 6.11. As for the two component system, the second law model in this case predicts a somewhat higher level of dispersion than the first law model, most

noticeably at the mole fraction peaks. In general, the results of the two models are quite similar.

The second law model with the multiple step function initial condition is found to over-predict dispersion for all configurations tested here. The piecewise linear initial condition model is found to predict higher levels of dispersion for the $D = 10^{-2}$ cm²/s runs, but produces identical results to the first law model when the smaller dispersion coefficient is used.

6.1.3. SECOND LAW DISPERSION MODEL: FRONT TRACKING ALGORITHM

The final model tested is the front tracking dispersion model. As described in Chapter 5, the only additional information required to run the front tracking model is the number and location of the fronts, the initial compositions upstream and downstream of the fronts and a mole fraction tolerance used for locating the starting and ending points of the profile for the dispersion calculation. Due to the nature of the transmissibility adjustment calculation, the interface compositions may at times be set considerably higher than the average block composition. To avoid computational problems created by attempting to remove more moles of a component from a grid block than exist in that block at the start of the time step, the mole fraction tolerance cannot be set as low as that used for the previous models. Values on the order of 0.1 to 4% have been used successfully; the runs reported here have been performed with a tolerance of 2%.

Initial tests were performed using the front tracking model in conjunction with the two point upstream weighting technique. These were done in an attempt to minimize numerical dispersion for those grid blocks which fall outside of the region being modified by the front tracking model. The calculated profiles for these cases were found to have

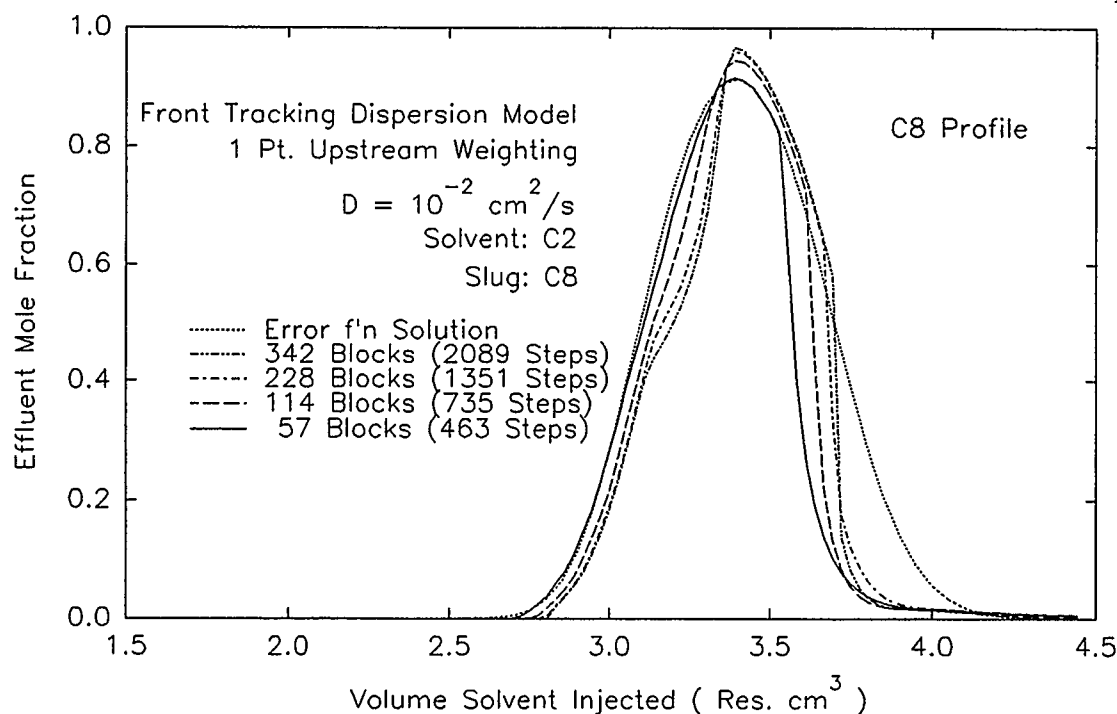


Figure 6.12: Taylor Experiment Simulation, Ethane + n-Octane, Second Law Front Tracking Dispersion Model with $D = 10^{-2} \text{ cm}^2/\text{s}$

inflections, flat spots or even oscillations in places. The runs reported here were thus all performed using the single point upstream weighting technique.

The ethane + n-octane system was simulated first using the same configurations of 114, 228 and 342 grid blocks, as well as a 57 block model which corresponds to 8 grid blocks for the original oil slug. The results for these runs are shown in Figure 6.12. For all the runs with this model, a much higher number of time steps were required as compared to the other models. This resulted in run times of 1, 3, 12 and 26 min for configurations with 57, 114, 228 and 342 grid blocks respectively on the rs6000.340 platform. All of the calculated profiles show close agreement with the error function profile for the initial portion of the leading edge.

A common feature in all of the profiles is the inflection point in the leading edge, although this inflection is not as noticeable for the 57 grid block model. This is the result

of the symmetrical region requirement on the calculated dispersion profile. When the leading edge of a profile contacts the end boundary of the model, the region of the trailing edge of the profile available for the dispersion calculation is reduced to maintain symmetry of the profile. For the first front, which makes up the leading edge of the entire profile plotted in the figure, the inflection point occurs when the midpoint of the front moves past the end of the reservoir and the dispersion calculation ceases for that front. The abrupt cutoff seen in the trailing edge of the profile is the result of interaction between the two front-tracking calculations. In order to avoid having the interface compositions for a given block calculated from two different profiles, the second profile is restricted to ensure that the domain for its calculation does not interfere with the domain for the first profile. This factor, combined with the symmetrical domain restriction, results in errors in the calculation of the second profile.

This calculation scheme shows good results for the location of the leading edge of the profile, even with a small number of grid blocks. Clearly, it cannot be used when two fronts are near enough to each other that interactions between the two will be taking place. Further results using this model for single front applications are included in the following two sections.

6.1.4. DISPERSION MODEL SUMMARY FOR THE TAYLOR DISPERSION EXPERIMENT SIMULATIONS

Due to excessive run times, it was not feasible to use the single point upstream weighting technique for this problem geometry and therefore use of the two point weighting method for numerical dispersion control is implicit in the results summarized here. The first law and second law piecewise linear models proved most capable of simulating the level of dispersion observed in the Taylor dispersion experiments. When a

process with a lower level of dispersion is simulated, the accuracy of the results depends more strongly on the number of grid blocks used in the simulation. The second law multiple-step dispersion model was found to greatly over predict the dispersion level with both dispersion coefficients tested. The front tracking model was found to perform adequately for the leading edge of the profile, however interactions between the two front tracking calculation regions resulted in unpredictable results for the second profile.

6.2. VISUAL EXPERIMENT SIMULATION

As outlined in the introduction, the visual experiment apparatus was designed by Sibbald and co-workers (1991) to observe the process of live reservoir oil and fully miscible solvent mixing in the absence of external temperature and pressure gradients. This absence of pressure gradients precludes the use of conventional compositional simulators for modeling the experiment, as there are no driving forces for the convection equation. This section describes modeling efforts combining the compositional simulator with the dispersion models developed in Chapter 5.

The equipment consisted of a glass tube of rectangular cross-section, 1 x 5 mm x 30 cm in length, with a notch drilled in one side at the midpoint. The tube was placed in a water bath at reservoir temperature and pressure. Live oil was pumped in one end of the tube until it reached the midpoint, displacing water through the notch into the surrounding vessel. Solvent was then injected slowly into the opposite end of the tube until all of the water was displaced through the notch and the gas and oil surfaces came into contact. This system is modeled as a rectangular tube initially containing solvent in one half and oil in the other, with contact between the phases at the midpoint. A constant pressure solvent injector, constrained at the initial pressure of the system, is positioned at the solvent end of the tube, and a similar oil injector is positioned at the other end. The tube length is set to

80 cm to avoid end effects interfering with the profile generation. The permeability is determined in a similar manner to that described for the Taylor dispersion experiment in Chapter 2. In this case, an analogy is drawn between the pressure drop equation for flow in a narrow slit of width W and thickness $2B$ (Bird et. al., 1960; p. 62):

$$Q = \frac{2 B^3 W \Delta P}{3 \mu \Delta x}$$

$$\frac{Q}{A} = \frac{B^2 \Delta P}{3 \mu \Delta x} \quad (6.1)$$

and Darcy's law:

$$\frac{Q}{A} = \frac{k \Delta P}{\mu \Delta x} \quad (6.2)$$

resulting in the permeability being defined as:

$$k = \frac{B^2}{3} \quad (6.3)$$

Again, the ethane solvent and n-octane or 5 component oil models will be used for the simulations. The physical parameters for the model are shown in the following table.

Table 6.2: Parameters for Visual Experiment Simulation

Length	$x = 80$ cm
Initial Solvent Zone	$0 < x < 40$ cm
Initial Oil Zone	$40 < x < 80$ cm
Height	$\Delta z = 1$ mm
Width	$\Delta y = 5$ mm
Porosity	100%
Permeability	8.3333×10^4 darcy
Pressure	25.2 MPa
Temperature	373.15 K

6.2.1. FIRST LAW DISPERSION MODEL

As for the Taylor dispersion experiments, the effects of grid block sizing and numerical dispersion control schemes are investigated for each of the physical dispersion models. The information reported by Sibbald et. al. (1991) showed that dispersion coefficients on the order of 0.1 to 1.0 cm²/s were observed in the visual experiment apparatus. The models are tested here with a value of $D = 1.0$ cm²/s and are run for 40 s with process variables recorded every 2 s. The majority of the results are presented as plots of solvent mole fraction vs. tube length at the termination time of the experiment.

The first model runs were performed for the ethane + n-octane system using the first law model with single point upstream weighting on model configurations of 20, 40 and 80 grid blocks. The minimum mole fraction tolerance for the dispersion calculation is again set to 10^{-8} , and the maximum time step size is set to 2 s in correspondence with the

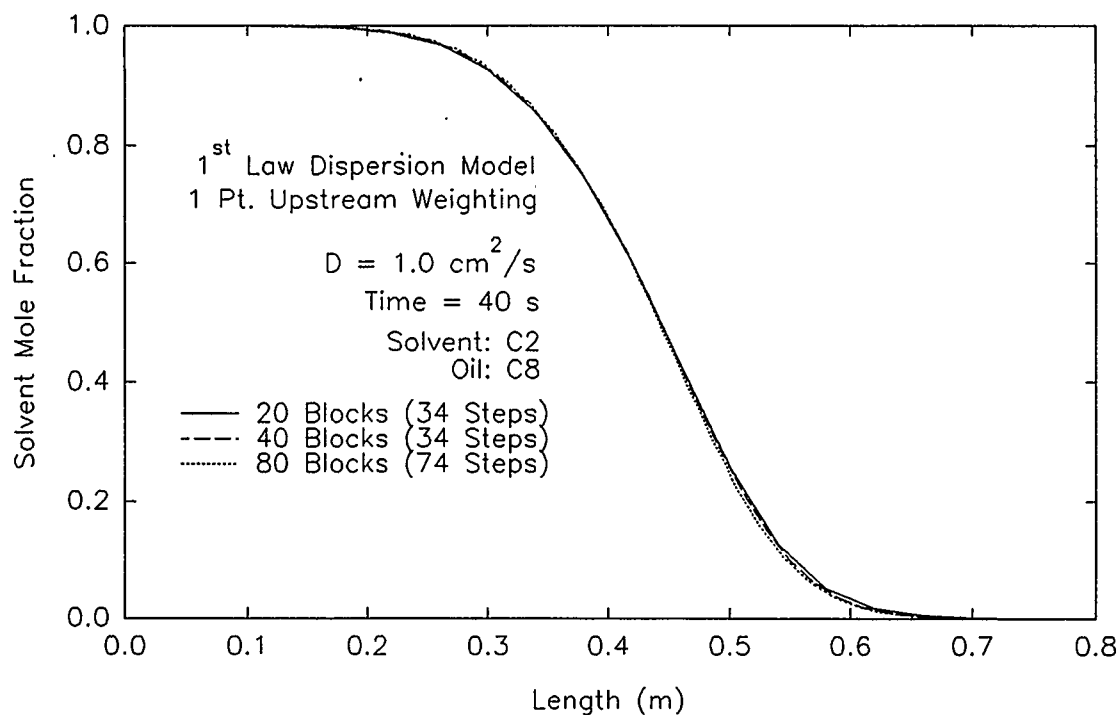


Figure 6.13: Visual Experiment Simulation, Ethane + n-Octane, First Law Dispersion Model with Single Point Weighting

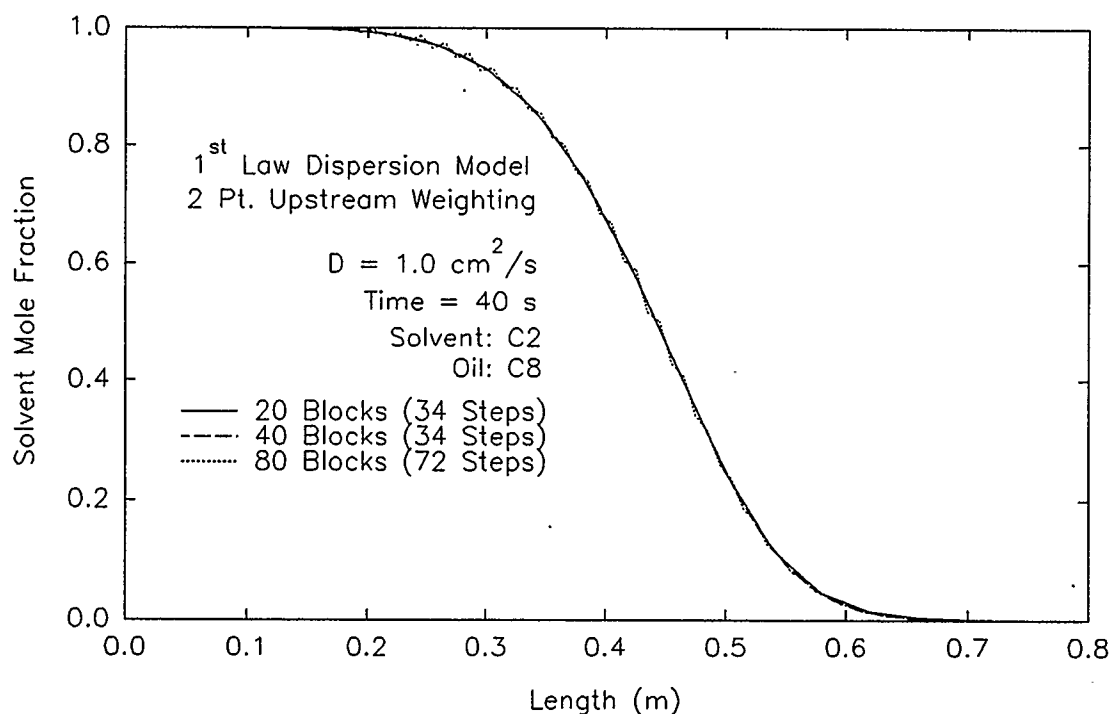


Figure 6.14: Visual Experiment Simulation, Ethane + n-Octane, First Law Dispersion Model with Two Point Weighting

process variable output frequency. The resulting profiles are shown in Figure 6.13. The three profiles are nearly identical; the 80 grid block model profile shows some slight oscillations that are not visible in the other solutions. The 20 and 40 block models both require 34 time steps to complete, resulting in run times of 2.9 and 3.1 s respectively on the rs6000.340 platform. The 80 grid block model requires 74 time steps for a run time of 16.1 s. Very similar results are observed for the model runs using the two point upstream weighting technique, the only difference being a somewhat more pronounced oscillation in the 80 grid block model profile. These results are shown in Figure 6.14.

It should be noted that these profiles are asymmetrical about the initial interface position at 0.4 m because the solvent is more mobile than the oil. When the volume of the mixed zone decreases, more fluid flows from the solvent side of the tube to the center than from the oil side, resulting in the profile being shifted towards the oil side of the midpoint.

6.2.2. SECOND LAW DISPERSION MODEL: APPROXIMATE INITIAL CONDITIONS

The second law dispersion model is tested for the same configurations as the first law model. The results obtained using the multiple step function initial condition are shown in Figure 6.15 for the single point upstream weighting case. For these model configurations, the profiles obtained with the two point and single point weighting techniques are indistinguishable, thus only one set of results is given.

All configurations required 34 time steps for this model, giving run times of 2.3, 4.6 and 8.8 s for the 20, 40 and 80 grid block runs respectively. This model predicts higher levels of dispersion for all configurations than the first law model, with the 80 block run coming closest to the previous predictions. Much more variation in the results with grid block numbers is also noted. As for the Taylor dispersion experiment simulations, this is

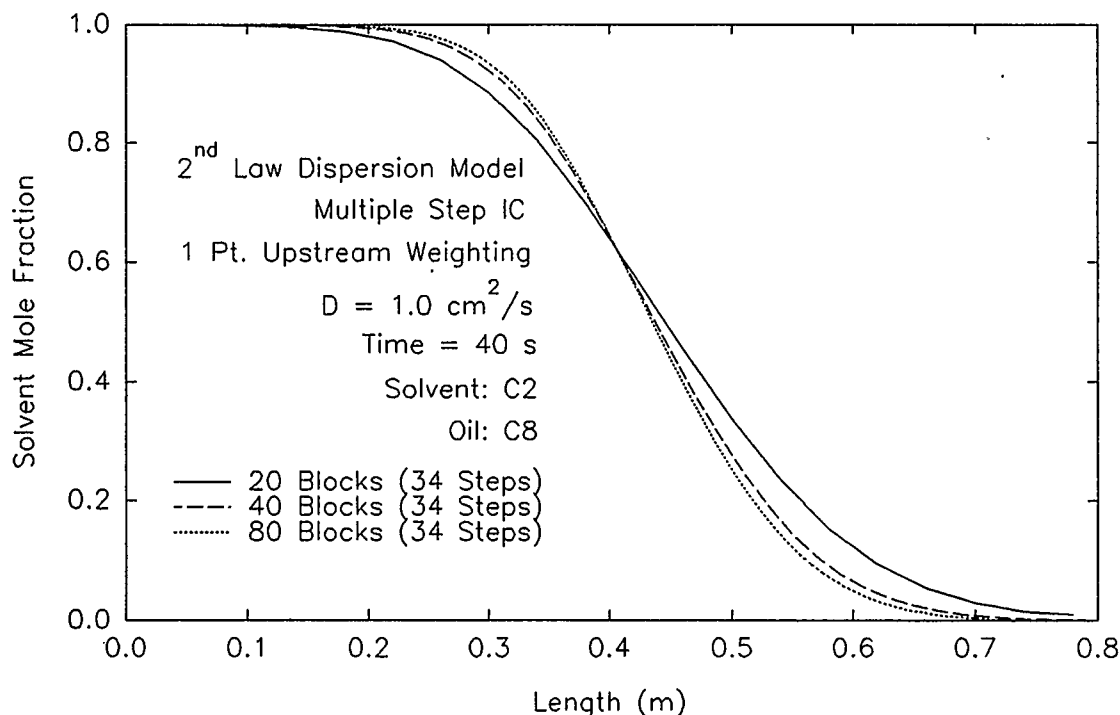


Figure 6.15: Visual Experiment Simulation, Ethane + n-Octane, Second Law Multiple Step Dispersion Model with Single Point Weighting

the result of the steps in the initial condition generating high levels of dispersion, even with the small time step sizes. The oscillations detected in the 80 block run of the first law model were not evident in this case.

The second law model using the piecewise linear initial condition was tested next; the results are shown in Figure 6.16. With this model, the three profiles are again nearly identical, the level of dispersion is similar to that predicted by the first law model, and no oscillations are observed in any of the solutions. Again, 34 time steps are required for the completion of each model run, resulting in run times of 2.4, 4.9 and 9.4 s for the 20, 40 and 80 grid block runs on the rs6000.340.

6.2.3. SECOND LAW DISPERSION MODEL: FRONT TRACKING ALGORITHM

Finally, these model configurations are tested with the front tracking algorithm.

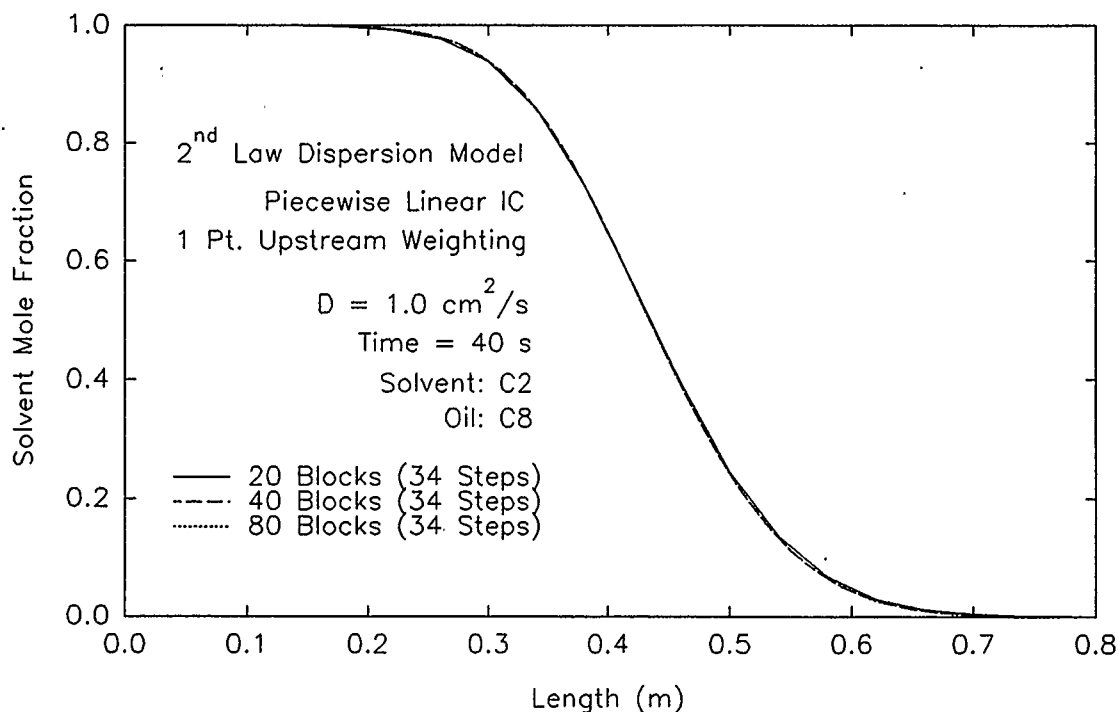


Figure 6.16: Visual Experiment Simulation, Ethane + n-Octane, Second Law Piecewise Linear Dispersion Model with Single Point Weighting

Results obtained with the two point and single point versions were essentially identical thus only one set of results is discussed here. The simulated profiles are shown in Figure 6.17. The profiles in this case are characterized by a single oscillation or inflection near the front midpoint for all configurations. The initial third and final third of the profiles lie close to the positions predicted by the other dispersion models. As for the other models, these all require 34 time steps to run to completion, with run times of 1.5, 3.6 and 6.9 s on the rs6000.340.

The oscillations result from the calculation of the interface composition from the profile determined as the solution of the error function. At the start of the simulation, the front midpoint will move to the right as more solvent is injected into the system. The composition at all block interfaces will be determined by integration of the portion of the profile located on the left side of the interface as long as the front midpoint is moving to

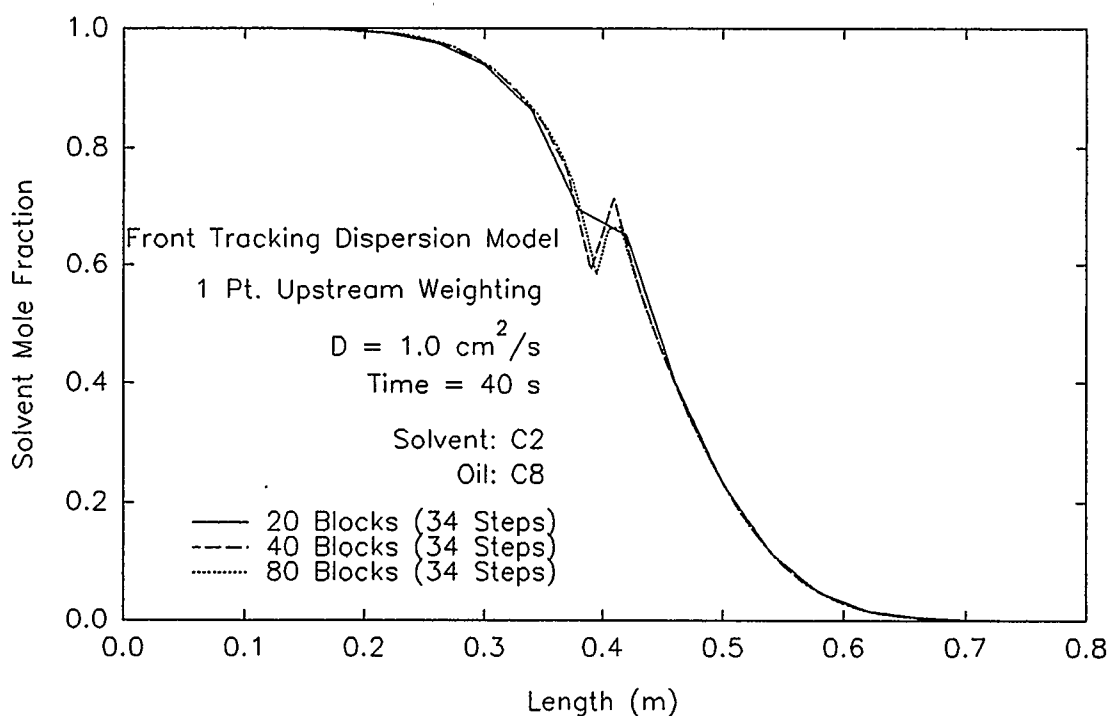


Figure 6.17: Visual Experiment Simulation, Ethane + n-Octane, Second Law Front Tracking Dispersion Model with Single Point Weighting

the right. This can lead to inconsistencies. Since fluid is being injected from both ends of the tube, the bulk movement of fluid across an interface may be in the opposite direction to the movement of the front midpoint. In its current form, the front tracking dispersion model cannot handle situations of this type, and is strictly applicable only when the bulk movement of the entire front is in a single direction.

6.2.4. DISPERSION MODEL SUMMARY FOR THE VISUAL EXPERIMENT SIMULATION

The original experimental results obtained from the visual apparatus shown by Sibbald et. al. (1991) include plots of the oil/solvent interface position vs. time. It was the "root of time" shape of these curves that lead to their characterization by dispersion coefficients. A plot of various solvent iso-concentration lines has been made from the results of the 80 grid block configuration of the second law piecewise linear initial condition dispersion model. The curves are generated by locating the position of the desired solvent concentration by linear interpolation from the output data file at 2 s intervals. The plot is shown in Figure 6.18. The curves show the correct characteristic "root of time" shape, and also show that the leading edge of the solvent profile, the 2% through 10% curves, travels more quickly than the trailing edge. This illustrates the greater mobility of the solvent, allowing it to move more quickly into the oil side of the tube than the oil moves into the solvent side.

Finally, several runs were performed for the ethane + 5 component oil model system, using the optimum settings for each model determined from the previous runs. These are 40 grid block configurations for the first law and second law piecewise linear models, and 20 grid blocks for the front tracking model. The profiles calculated for this

system exhibit the same trends as the ethane + n-octane system. The results are shown in Figure 6.19.

For the visual experiment simulations performed here, the first law and second law piecewise linear models are found to give the most consistent results over the range of grid block configurations tested. Of these two, the second law piecewise linear model showed no tendency towards the oscillations that the first law model developed with the larger number of grid blocks. The second law multiple step model was found to over-predict the amount of dispersion unless a large number of grid blocks was used. The front tracking model has to be considered unsuccessful for use in the specialized situation in which there is the possibility that portions of the front will have different directions of bulk movement. In terms of simulation running times, the models ranked from fastest to slowest are: front tracking model, first law, second law multiple step and second law

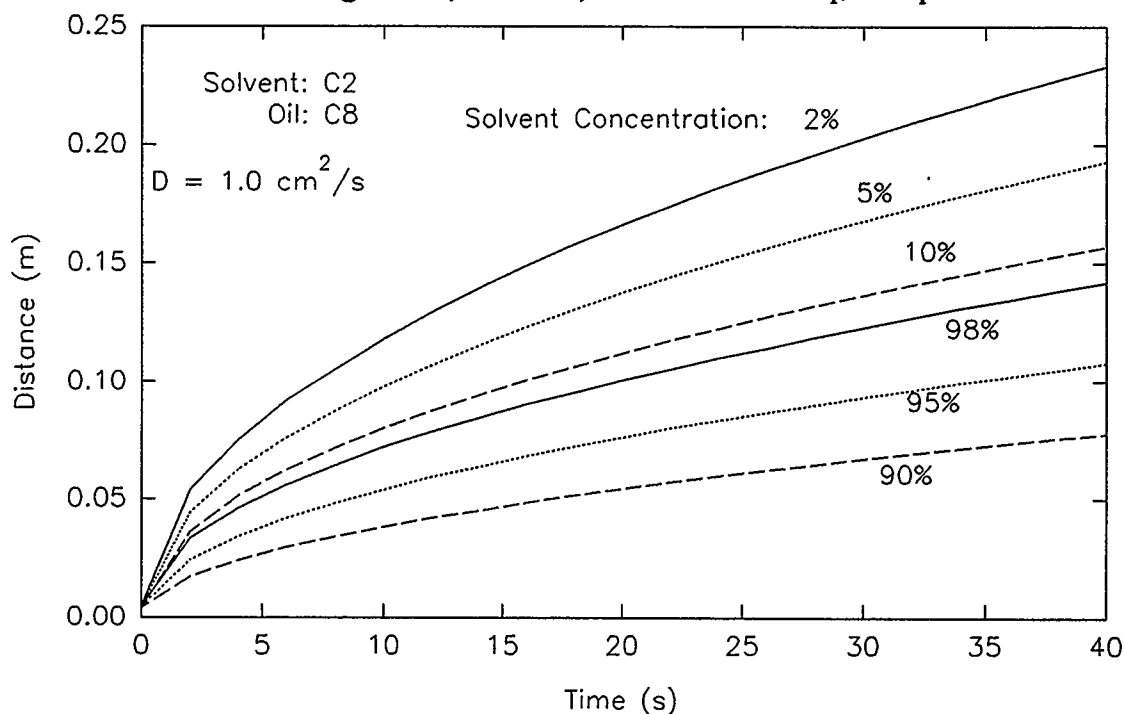


Figure 6.18: Solvent Isoconcentration Line Movement in the Visual Experiment Simulation

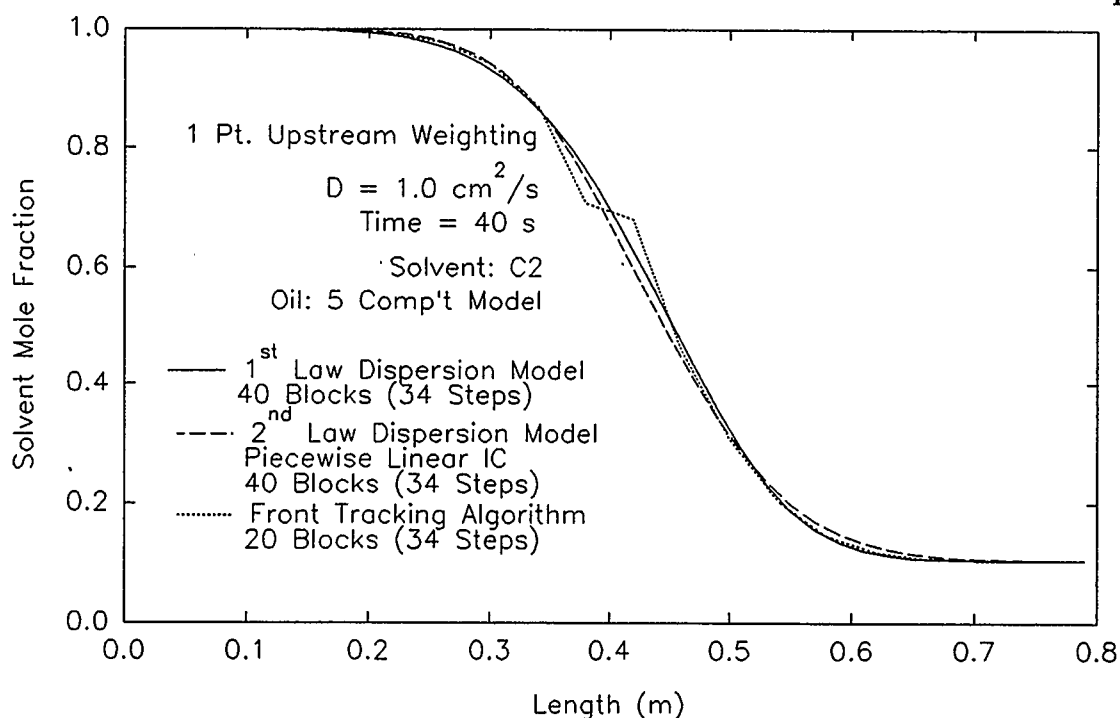


Figure 6.19: Visual Experiment Simulation, Ethane + 5 Component Oil, Dispersion Model Summary

piecewise linear. Although, for these simulations the differences in running times are small.

6.3. SLIM TUBE SIMULATION

The final one dimensional system tested is a standard slim tube experimental apparatus. This system will be modeled as a tube of square cross section, filled with some form of packing and initially saturated with oil. A constant rate solvent injector is positioned at one end of the tube and a constant back pressure production well is placed at the other end. The ethane solvent and n-octane or 5 component oil model systems will be used for these simulations as well. The same values of the dispersion coefficient will be used as for the Taylor dispersion experiment simulations, as they represent a possible level of enhanced dispersion for these fluids which exhibit a high negative volume change on mixing. The temperature and pressure of the Taylor dispersion experiment will also be used. The physical parameters used for the simulations are shown in the following table.

Table 6.3: Slim Tube Simulation Parameters

Length	$x = 12.15 \text{ m}$
Height and Width	$\Delta y = \Delta z = 0.42608 \text{ cm}$
Porosity	36.5%
Permeability	6.0 darcy
Pressure	22.75 MPa
Temperature	372.05 K
Solvent Injection Rate	7.06 mL/hr

6.3.1. FIRST LAW DISPERSION MODEL

As for the Taylor dispersion experiment simulation, the characteristics of the system must be investigated in order to specify a configuration which minimizes numerical dispersion yet allows reasonable run times. The first runs of the program were performed for the ethane + n-octane system with the dispersion model turned off. Configurations of 50, 100 and 200 grid blocks were used with the 2 point upstream weighting technique, and a 400 grid block model with single point upstream weighting was also investigated. The time step size controls are set to allow the simulator to select the maximum possible time steps, subject to the constraint that the process variable output frequency is set to 500 s. The results for all cases shown in this section are plotted as mole fraction at the effluent plotted vs. the pore volumes of fluid injected.

The results for these initial runs are shown in Figure 6.20. The 50 grid block model shows too much numerical dispersion to be useful in evaluation of the physical dispersion models; the other three configurations will be used so that the effects of number of grid blocks and numerical dispersion controls on the dispersion models can be investigated. The 200 block configuration with 2 point weighting shows the lowest level of numerical dispersion, followed by the 400 block single point model and finally the 100 block two point model.

The initial test of the first law dispersion model is done with the 100, 200 and 400 grid block models described above for a dispersion coefficient of $D = 10^{-2} \text{ cm}^2/\text{s}$. As for the Taylor dispersion simulations, an error function solution is generated as a comparison for the profiles calculated using the dispersion models with the simulator. Again, the error function solution cannot be considered an exact solution that the others should conform to, as it does not take into account any fluid shrinkage effects. The results of these runs are shown in Figure 6.21.

For each configuration, the number of time steps required to run to completion is approximately the same (within 10%) as for the runs with no dispersion model, thus the amount of numerical dispersion should be the same in each case. The models employing the two point upstream weighting show only a small increase in the total amount of dispersion when the physical dispersion model is added. As was seen before, the numerical

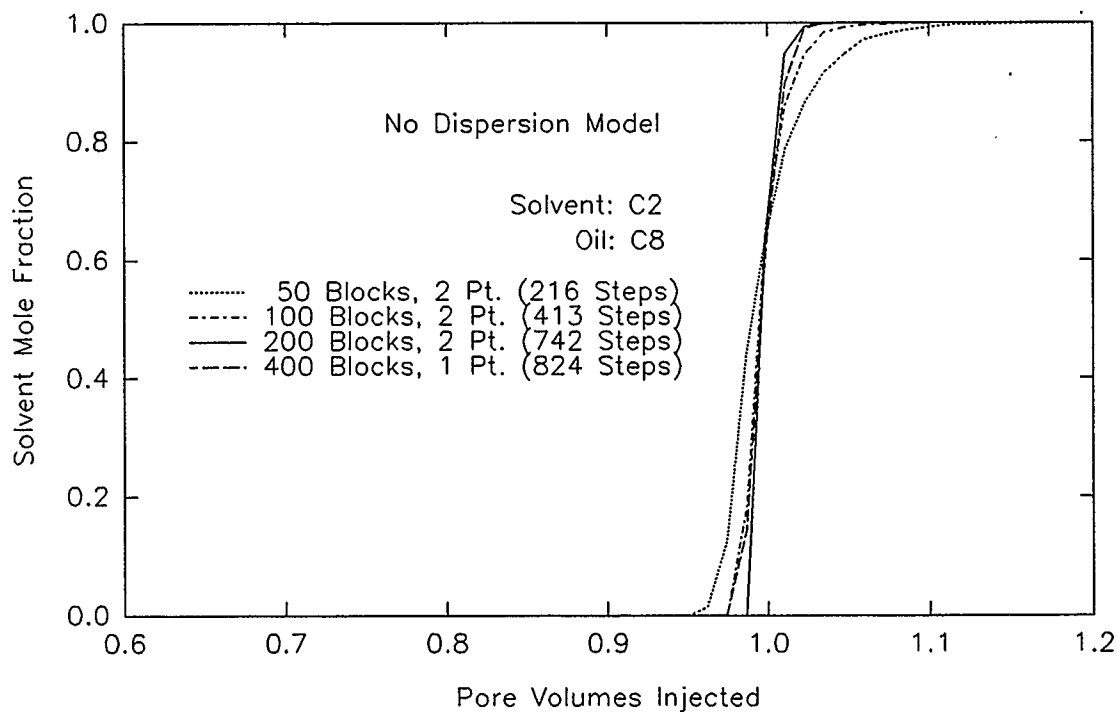


Figure 6.20: Slim Tube Simulation, No Dispersion Model

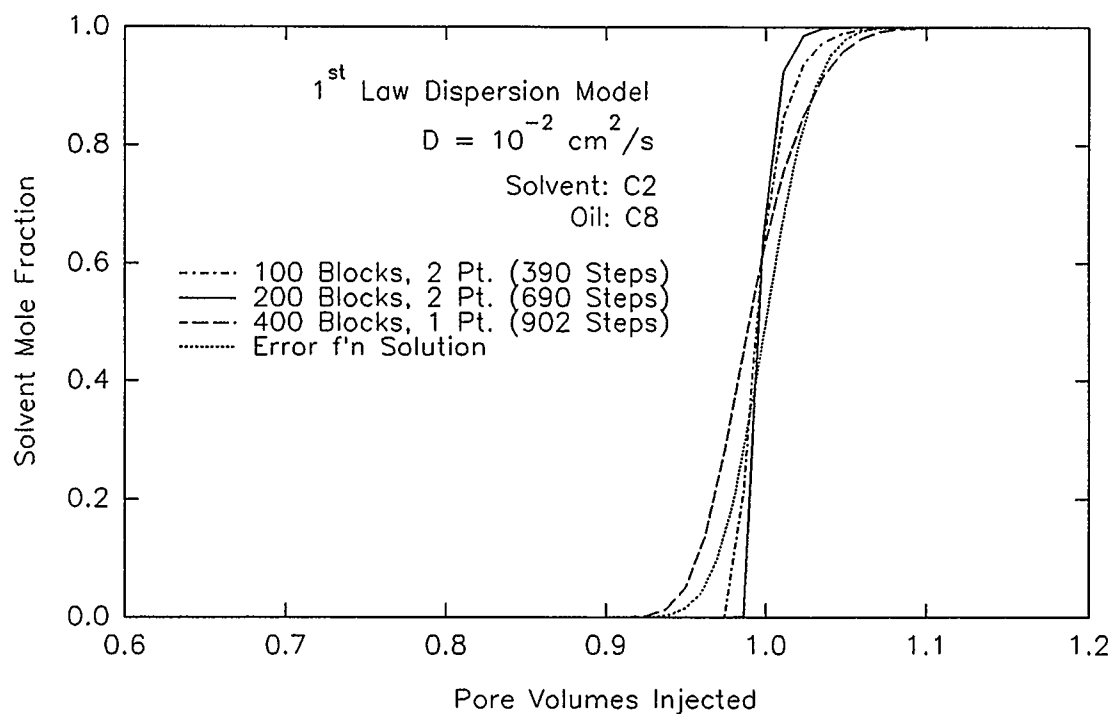


Figure 6.21: Slim Tube Simulation, First Law Dispersion Model, $D = 10^{-2} \text{ cm}^2/\text{s}$

dispersion control also acts to reduce physical dispersion present in the simulation. The single point model, however, appears to give a more realistic level of dispersion in comparison to the error function solution. The run times on the rs6000.320h for these models are 2.7, 8.8 and 30.5 min for the 100, 200 and 400 block cases respectively.

The same runs were performed next with the dispersion coefficient set to $D = 10^{-3} \text{ cm}^2/\text{s}$; the results are shown in Figure 6.22. The differences between the profiles for all configurations calculated in this case and those calculated with no dispersion model at all are extremely small. As this level of dispersion is so close to that already present due to numerical dispersion, the physical dispersion models have negligible effects on the profiles.

The model is tested next on the ethane + 5 component oil system. The base case with no dispersion model is run for the 100, 200 and 400 grid block models. The profiles

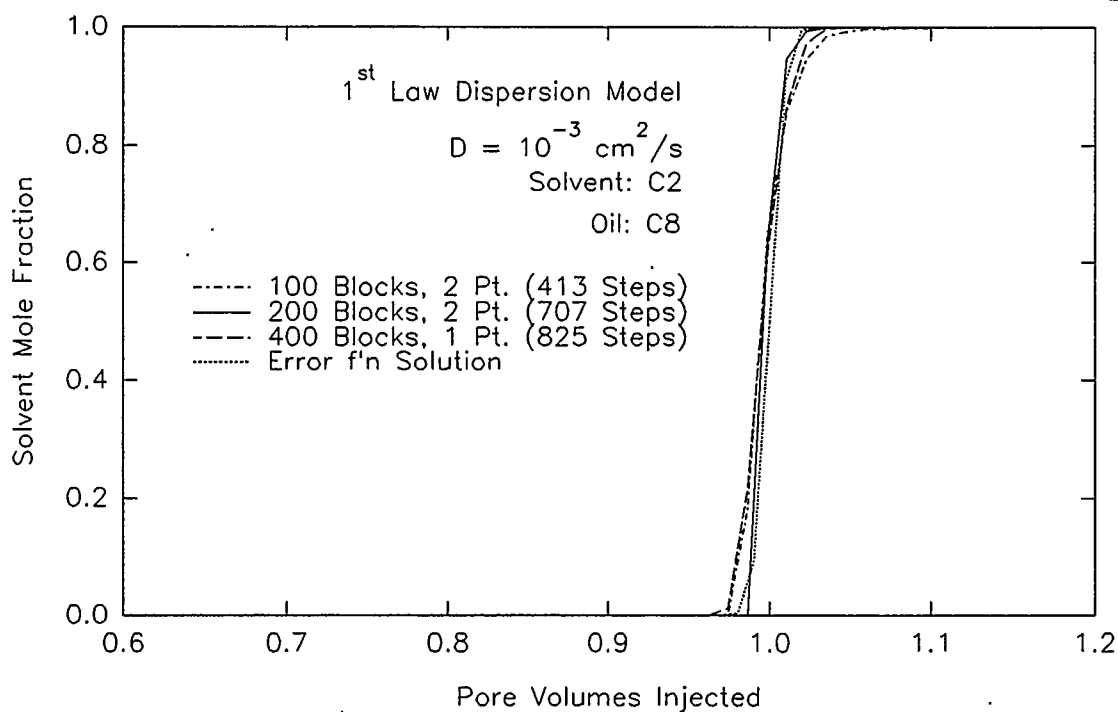


Figure 6.22: Slim Tube Simulation, Ethane + n-Octane, First Law Model, $D = 10^{-3} \text{ cm}^2/\text{s}$

are similar to those obtained for the ethane + n-octane case, however the 400 block model with single point weighting appears to have a more greatly dispersed solvent profile in the multicomponent case than for the two component case. These results are shown in Figure 6.23, along with the results obtained for this system using $D = 10^{-2} \text{ cm}^2/\text{s}$.

As for the ethane + n-octane case, the two point weighting technique reduces the physical dispersion to such a degree that the total dispersion is almost identical to that obtained with no physical dispersion model at all. For the 400 block model with single point weighting, the dispersion model has a significant effect. The number of time steps required to complete the runs is reduced somewhat when the dispersion model is employed as the pressure equation is more easily solved when the fronts are more diffuse; the change in number of time steps is small enough, however, that it should have little

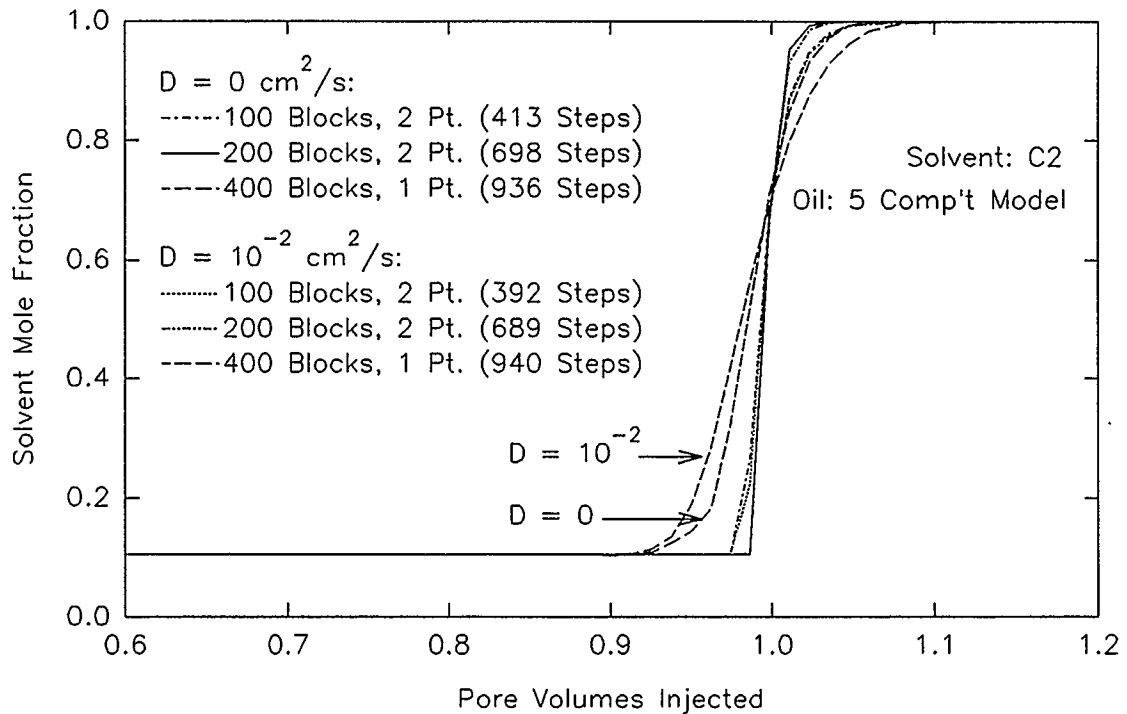


Figure 6.23: Slim Tube Simulation, Ethane + 5 Component Oil

effect on the degree of numerical dispersion present for the no dispersion and dispersion model cases.

The results of these simulations indicate that for this slim tube geometry, the use of numerical dispersion control also limits the physical dispersion introduced by the first law model, thereby under predicting the dispersion of the front. When single point upstream weighting is used, the physical dispersion model can correctly predict the dispersion of the front, however, the numerical dispersion problem can only be countered by using fine grids and optimal time step sizes.

6.3.2. SECOND LAW DISPERSION MODEL: APPROXIMATE INITIAL CONDITIONS

The second law dispersion model is tested first with the multiple step initial condition. Again the minimum mole fraction tolerance for carrying out the dispersion calculation is set to 10^{-8} and the simulator is configured to select the maximum possible time steps. The profiles calculated for the ethane + n-octane system with $D = 10^{-2} \text{ cm}^2/\text{s}$, using the model configurations as in the previous section, are shown in Figure 6.24.

In this case, the 400 grid block model with no numerical dispersion control (single point weighting) has greatly over predicted the amount of dispersion in the system. The configurations employing the two point upstream weighting technique produce profiles which approximate that given by the error function, however, their shape is a strong function of the number of grid blocks used. The final shape of these profiles is the result of

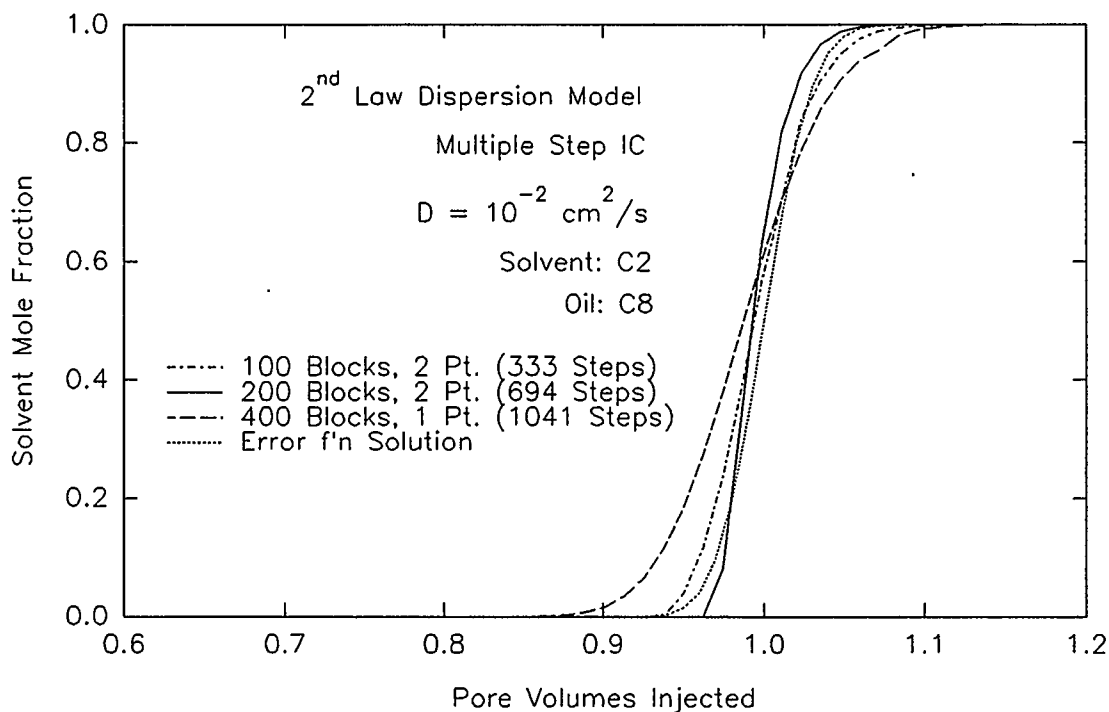


Figure 6.24: Slim Tube Simulation, Second Law Multiple Step Dispersion Model,
 $D = 10^{-2} \text{ cm}^2/\text{s}$

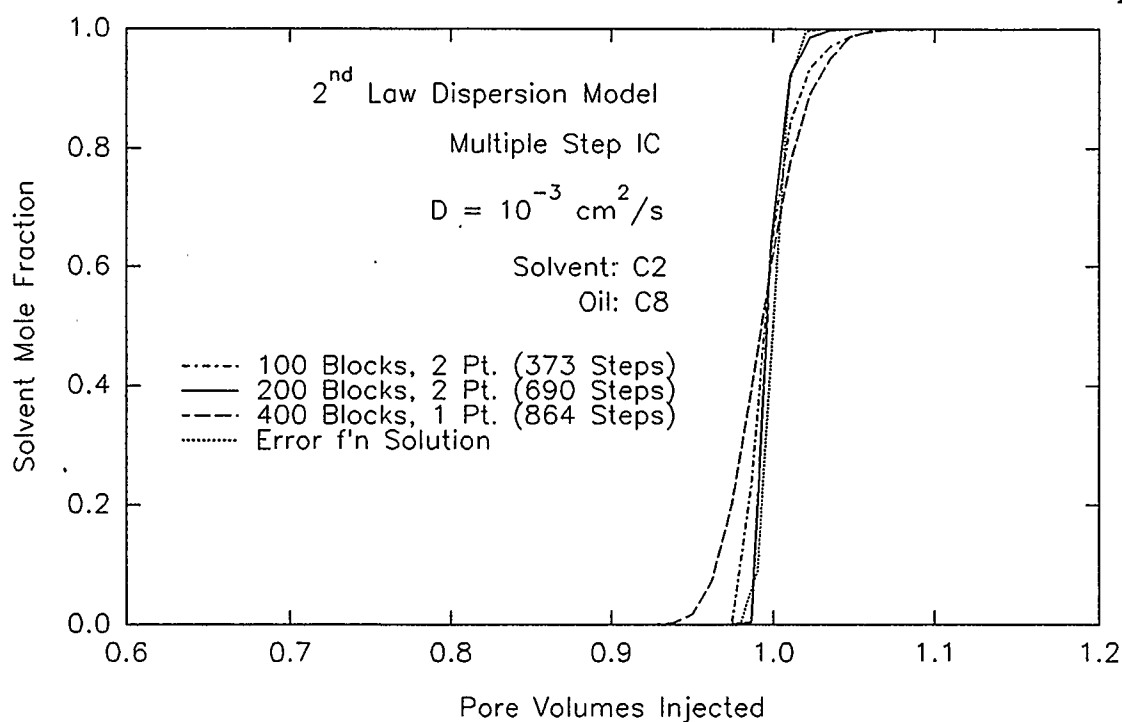


Figure 6.25: Slim Tube Simulation, Second Law Multiple Step Dispersion Model,
 $D = 10^{-3} \text{ cm}^2/\text{s}$

the multiple step function dispersion model over-predicting the level of dispersion, and the two point weighting technique reducing the total dispersion generated as numerical and physical dispersion. The run times on the rs6000.320h were 2, 9, and 46 min for the 100, 200 and 400 block models.

The results of the calculation for these models using $D = 10^{-3} \text{ cm}^2/\text{s}$ are shown in Figure 6.25. In this case the 100 and 400 block models over-predict the amount of dispersion, and the 200 block model approximates the error function profile only by virtue of having the correct amount of numerical dispersion.

The second law piecewise linear dispersion model is examined next, using the same model configurations and simulator parameters as for the multiple step model. The calculated profiles for the ethane + n-octane system using $D = 10^{-2} \text{ cm}^2/\text{s}$ are shown in Figure 6.26. For the models employing the two point upstream weighting technique, the

profiles are identical to those calculated with the first law model. The 400 block single point configuration shows slightly more dispersion with this model than with the first law model. As for the first law model, the numerical dispersion control scheme counters the effect of the physical dispersion model. Run times for this model were 2, 7 and 23 min for the 100, 200 and 400 block models on the rs6000.340.

The runs for $D = 10^{-3} \text{ cm}^2/\text{s}$ were performed with this model as well; the results are shown in Figure 6.27. As expected the results are essentially identical to those generated from the first law model. One point of interest is that the profiles calculated using the two point upstream configuration with the multiple step and the piecewise linear model variations are nearly identical when $D = 10^{-3} \text{ cm}^2/\text{s}$, yet show significant differences when $D = 10^{-2} \text{ cm}^2/\text{s}$. This shows that the numerical dispersion control scheme reduces physical dispersion effects when they are below a certain magnitude, but will not eliminate

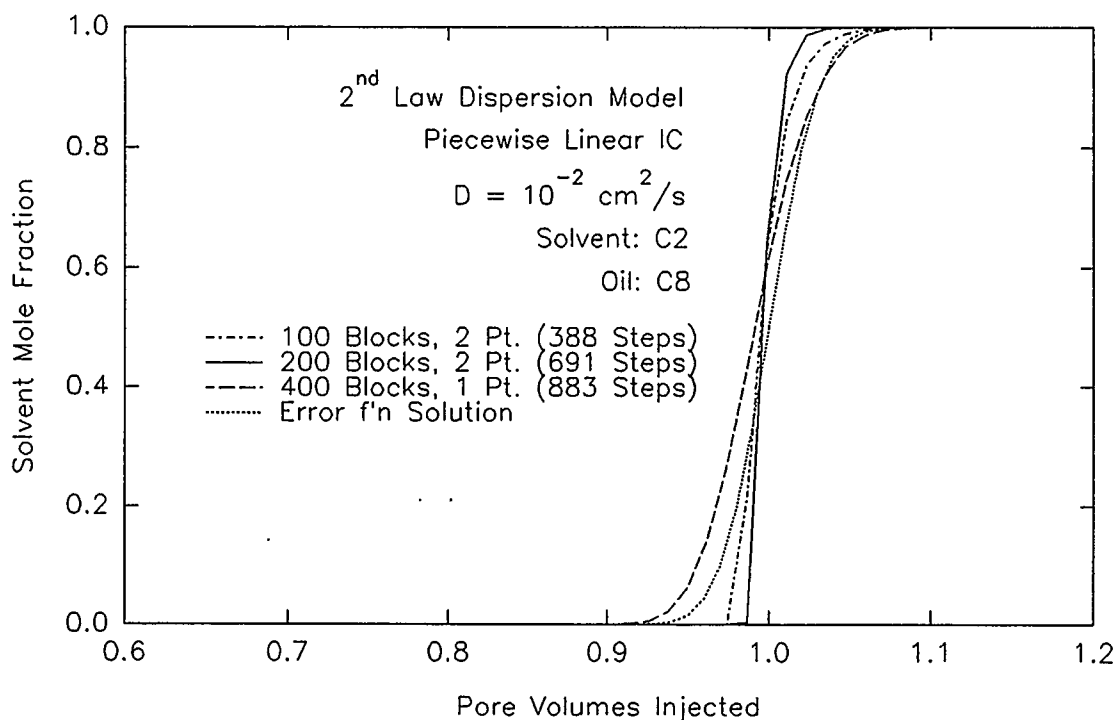


Figure 6.26: Slim Tube Simulation, Second Law Piecewise Linear Dispersion Model, $D = 10^{-2} \text{ cm}^2/\text{s}$

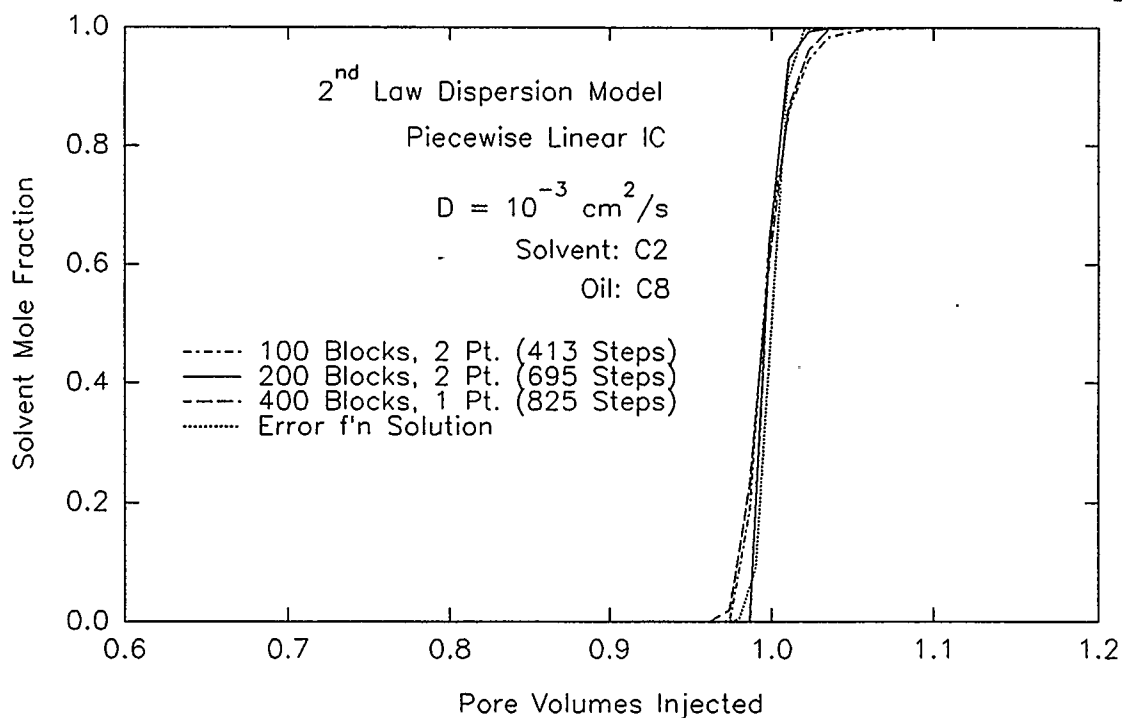


Figure 6.27: Slim Tube Simulation, Second Law Piecewise Linear Dispersion Model, $D = 10^{-3} \text{ cm}^2/\text{s}$

very high levels of physical dispersion.

6.3.3. SECOND LAW DISPERSION MODEL: FRONT TRACKING ALGORITHM

Finally, the front tracking model is applied to the slim tube model simulation. As described in the Taylor dispersion experiment simulation section, the only additional information required for this model is the initial front location, the compositions upstream and downstream of the front, and the mole fraction tolerance for locating the starting and ending points of the profile. The initial front location is at $x = 0$, the injection point for the tube; the upstream composition is thus the composition of the solvent being injected and the downstream composition is that of the oil initially in the tube. The mole fraction tolerance is set at 2% as for the Taylor dispersion simulations.

The front tracking model is tested for configurations of 25, 50, 100 and 200 grid blocks. The initial test is done with the two point upstream weighting technique for the ethane + n-octane system with $D = 10^{-2} \text{ cm}^2/\text{s}$. The results of these runs are shown in Figure 6.28. The 25 block model apparently gives insufficient resolution for this problem, however the position of leading edge of the profile compares well with that obtained for the 400 block single point model configuration using the first law or second law piecewise linear models. The other three profiles approximate the error function profile reasonably well, although the tailing of the trailing edge of the profile is a strong function of the number of grid blocks used. Calculation times ranged from 0.5 to 20 min on the rs6000.320h workstations.

These calculations are repeated with the same system configurations but with the single point upstream weighting technique. These results are shown in Figure 6.29.

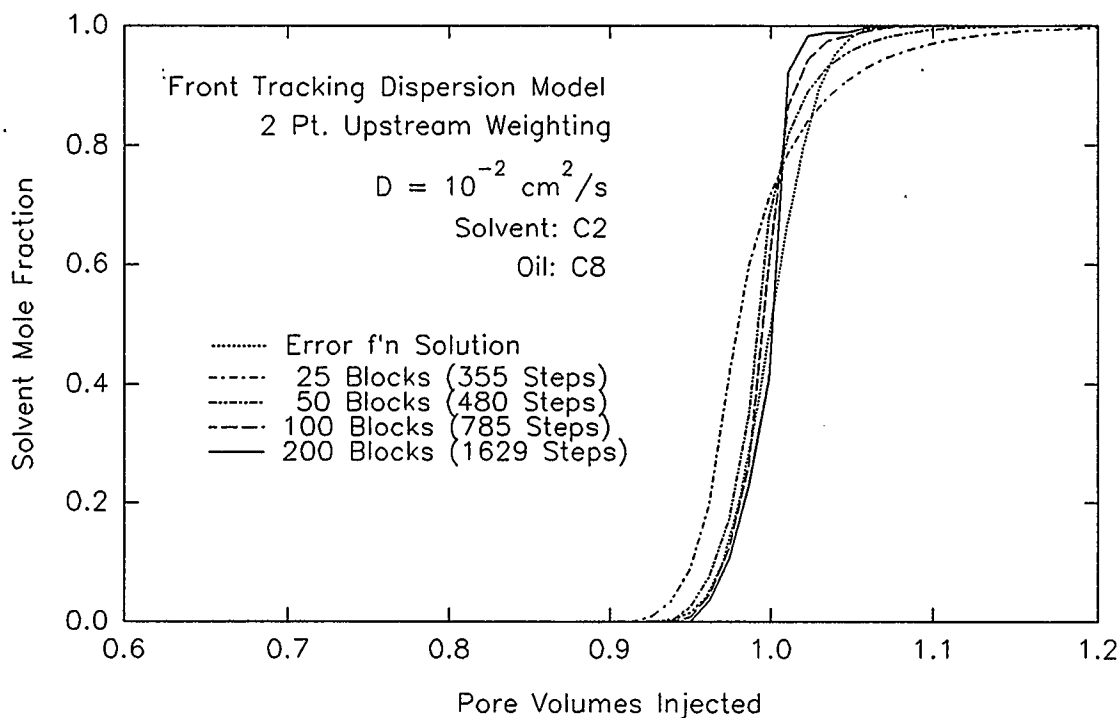


Figure 6.28: Slim Tube Simulation, Front Tracking Dispersion Model, Two Point Weighting with $D = 10^{-2} \text{ cm}^2/\text{s}$

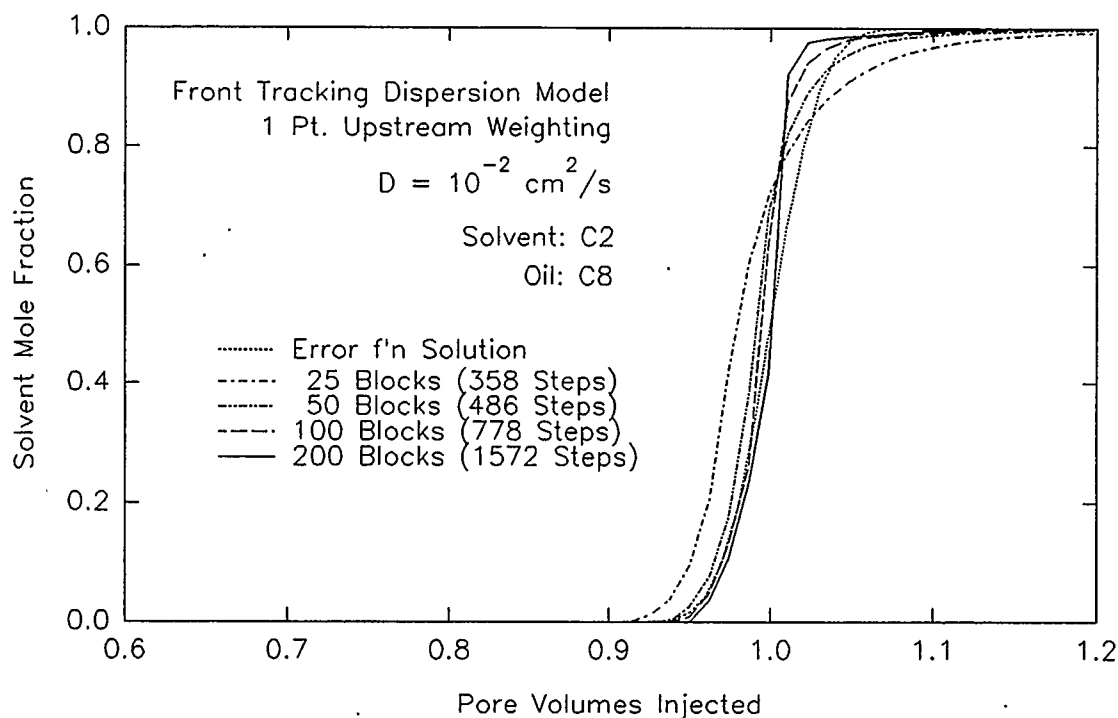


Figure 6.29: Slim Tube Simulation, Front Tracking Dispersion Model, Single Point Weighting with $D = 10^{-2} \text{ cm}^2/\text{s}$

Although the interface mole fractions for the blocks over which the profile is calculated to be active are set according to the interface integration scheme and will not be affected by the normal single point or two point techniques, the blocks which fall outside of the dispersion calculation zone will affect the leading and trailing edge of the profile. In this case the single point scheme is seen to create more tailing off of the trailing edge of the profile. There is very little, if any, difference in the leading edges of the profiles.

The calculations are performed next using the same configurations for the ethane + n-octane system with $D = 10^{-3} \text{ cm}^2/\text{s}$. As the differences between the single point and two point cases described above were small, the single point technique is used for the remaining runs, as it required fewer time steps. The calculated profiles are shown in Figure 6.30. In this case again, the 25 block model has inadequate resolution to track the front. The other three configurations show good results as far as placing the leading edge of the

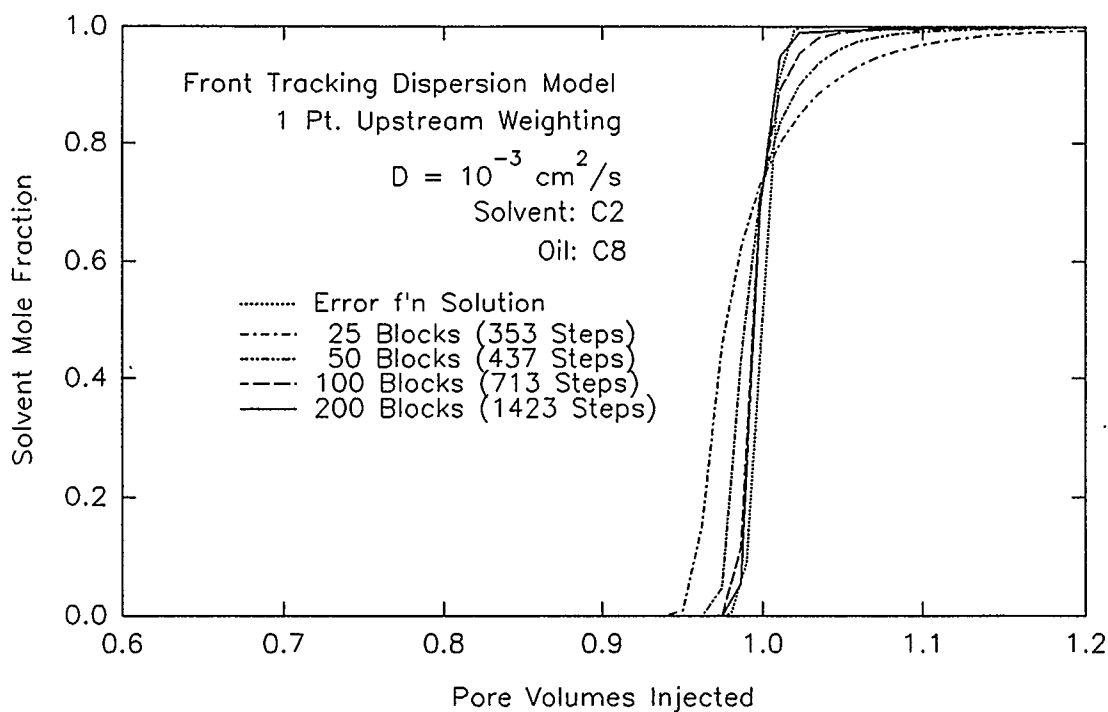


Figure 6.30: Slim Tube Simulation, Front Tracking Dispersion Model, Single Point Weighting with $D = 10^{-3} \text{ cm}^2/\text{s}$

profile, while only the 100 and 200 block models maintain enough control on the trailing edge of the profile. When the profiles are examined in terms of the number of blocks they extend over, however, even the 25 block model performs well, as the majority of the profile is contained within about 4 grid blocks.

Finally, the ethane + 5 component oil system is modeled using these model configurations and a dispersion coefficient of $D = 10^{-2} \text{ cm}^2/\text{s}$. The results are shown in Figure 6.31. The same trends regarding leading edge and trailing edge shape and placement are observed in this case as for the two component examples.

6.3.4. DISPERSION MODEL SUMMARY FOR THE SLIM TUBE SIMULATION

The runs with $D = 10^{-2} \text{ cm}^2/\text{s}$ yielded the following results. With the two point upstream weighting technique, the first law and second law piecewise linear models were

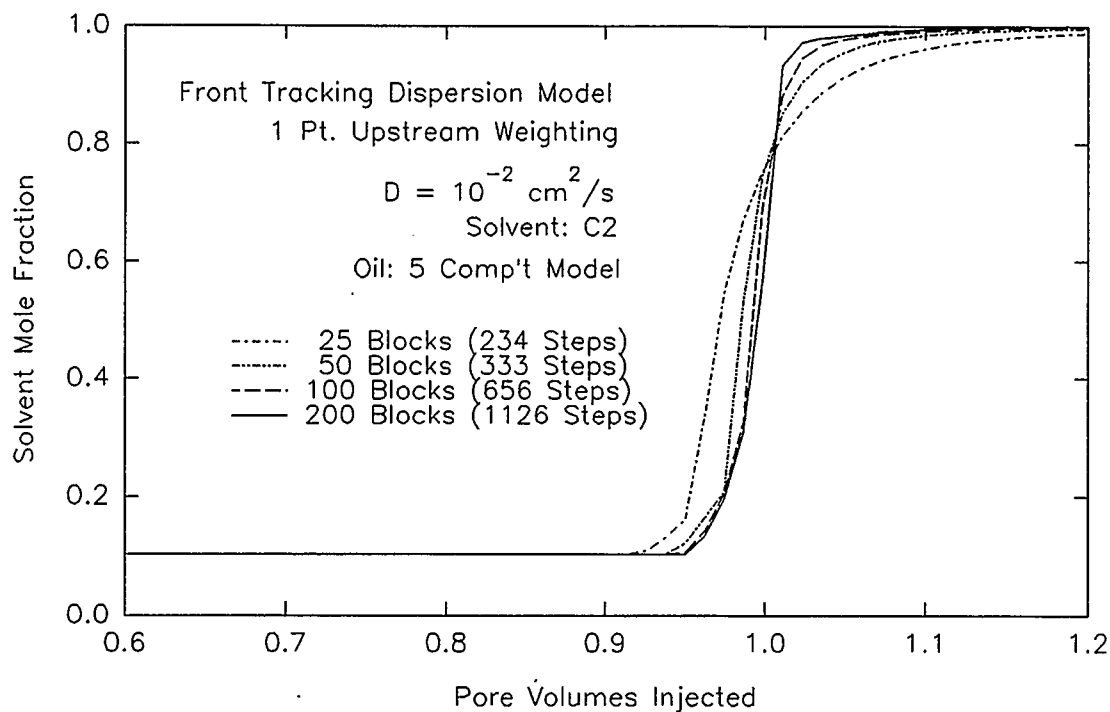


Figure 6.31: Slim Tube Simulation, Ethane + 5 Component Oil, Front Tracking Dispersion Model, Single Point. Weighting with $D = 10^{-3} \text{ cm}^2/\text{s}$

found to under-predict the level of dispersion. The second law multiple step dispersion model provided approximately the right magnitude of dispersion. For the single point runs, the first law and second law piecewise linear models were found to predict the level of dispersion correctly, while the second law multiple step dispersion model over-predicted the dispersion. The front tracking model allowed accurate calculation of the leading edge of the profile for a range of grid block refinements, and could predict the shape of the trailing edge as well with an adequate number of blocks.

7. CONCLUSIONS AND RECOMMENDATIONS

7.1. CONCLUSIONS

Three methods have been investigated for the modification of a conventional compositional simulator based on the convective flow equation to allow the explicit treatment of dispersive processes. The fundamental technique used for all three models is the addition of dispersive flow rates as source/sink terms in the convective flow equation. This approach has proved capable of modeling convective-dispersive processes within the framework of an IMPES type compositional simulator. Advantages of this approach over modeling with a full convection-dispersion equation include reduced computational costs and enhanced computational stability. Some conclusions drawn regarding the different dispersion models are:

1. The Fick's first law model as presented by Thiebot and Sakthikumar (1991) can be used to predict dispersion in a variety of systems in one, two or three dimensions. The total amount of dispersion predicted by this model will be the sum of the physical dispersion and numerical dispersion (truncation error); thus the dispersion prediction will depend on grid block refinement and time step sizes. Techniques used to limit numerical dispersion can also limit the amount of physical dispersion generated from the first law model. The results of the model increase in accuracy with increasing grid refinement and decreasing time step size.
2. The Fick's second law model developed in this work is derived as a one-dimensional technique, but can be applied as a series of one-dimensional calculations to rows of grid blocks in two or even three dimensions. The multiple step approximate initial condition applied with this model is found to over-predict the level of dispersion in cases involving large time steps and/or high dispersion coefficients. The piecewise linear approximate

initial condition used with this model is capable of modeling convective-dispersive processes in the three system geometries studied.

3. For some conditions, primarily for fine grids with low dispersion coefficients and small time step sizes, the results of the second law piecewise linear model coincide with those obtained using the first law model. However, for other conditions, the results diverge and this model can reflect interactions between gradients across two faces of a grid block or the changing concentration gradient across an interface over the course of a time step. This model also did not show any oscillations in the solution which occurred in some cases with the first law model.

4. The conclusions in 1, regarding numerical dispersion, also apply for the second law approximate initial condition models.

5. The second law front tracking model is applicable to systems of one dimension only. It is capable of locating the leading edge of a flowing dispersive front accurately even when a relatively coarse grid is used. The shape and location of the trailing edge of the profile is not as accurately predicted.

6. The front tracking algorithm is not as generally applicable as the other two models, failing to give good results in situations where two fronts are interacting, or when a weak or variable convective component of the flow exists.

7. The front tracking algorithm includes numerical dispersion control inherent within the calculation scheme, thus is not as sensitive to grid block and time step size variations.

7.2. RECOMMENDATIONS

The primary recommendation stemming from this work is that the degree of numerical dispersion in a model system must be well characterized before attempting to add a physical dispersion model. The ability of numerical dispersion control schemes to limit predicted physical dispersion must be taken into account.

The first law model and second law piecewise linear model show similar computation times and comparable results. The possible smoothing effects exhibited by the second law model may make it a more desirable choice. This second law scheme may also be extended to full two-dimensional solution of an approximate initial condition profile. The Green's function methodology can be used as described in Chapter 4 to derive an analytical expression for the concentration profile in two dimensions. As for the one-dimensional case, this profile can be integrated over a grid block to determine the number of moles of a component in that block, and the determination of dispersive flux to or from the block can be carried out using the methods given in Chapter 5. This would give the advantage of accounting for concentration gradients in both directions on the magnitude of dispersion. Since the calculation methodology would be the same as for the one dimensional model, the major difficulty in applying this method is in the definition of an integrable approximate initial condition in two dimensions. Multiple plane segments equal to the mole fraction in each block would lead to over-prediction of dispersion as in the multiple step one dimensional model. A piecewise planar analog to the piecewise linear initial condition would be required.

The second law front tracking dispersion model performed well for maintaining the definition of a front over a small number of grid blocks in a flowing system. Complications in the physical system as shown in this work, however, caused deterioration in the model

performance. Although field scale simulations require more than one dimension, a model of this type can be useful for laboratory simulations or situations in which dispersion in one direction is dominant. Increasing the sophistication of the interface composition calculation may improve the prediction of the trailing edge of the profile, for example by calculating the bulk movement of the front for each interface, rather than only for the front midpoint.

The equation of state calculations in this dissertation primarily affected the volumes of the flowing fluids, since at no point did the simulated reservoir conditions result in two equilibrium hydrocarbon phases. It would be of interest to pursue the dispersion model approach of this thesis in cases where phase separations occur, at least in some reservoir blocks. Some of the formalism required to do so has been outlined in Chapters 3 and 5 of this dissertation.

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APPENDIX
EXTENSION AND EVALUATION OF GREEN'S FUNCTION METHODS

A.1. ONE DIMENSIONAL LAPLACE DOMAIN SOLUTIONS

The Laplace domain solution procedure was outlined in Section 4.4.4 of this dissertation. The details of obtaining a solution for a specific boundary flux are described here. The flux function must be approximated numerically by a function with a known Laplace transform. This may be accomplished using a piecewise linear approximation. In this approach, the value of a function $F(t)$ is known for a number of values of t as shown in the following table.

t	$F(t)$	
T_0	$F(T_0) = F_0$	
T_1	$F(T_1) = F_1$	
$\vdots$	$\vdots$	
T_k	$F(T_k) = F_k$	
$\vdots$	$\vdots$	
T_N	$F(T_N) = F_N$	(A.1)

The original function is approximated by chords between these known points. The approximating function is defined by the following equations:

$$f_k(t) = F_{k-1} + \dot{F}_k(t - T_{k-1}) \quad T_{k-1} \leq t \leq T_k; k = 1, N \quad (\text{A.2})$$

$$\dot{F}_k = \frac{F_k - F_{k-1}}{T_k - T_{k-1}} \quad (\text{A.3})$$

As the function $F(t)$ defined in this way is piecewise continuous, it has a Laplace transform given by

$$\begin{aligned} \bar{F}(s) = & \int_{T_0}^{T_1} e^{-st} f_1(t) dt + \int_{T_1}^{T_2} e^{-st} f_2(t) dt + \dots + \int_{T_{k-1}}^{T_k} e^{-st} f_k(t) dt \\ & + \dots + \int_{T_{N-1}}^{T_N} e^{-st} f_N(t) dt + \int_{T_N}^{\infty} e^{-st} f_{N+1}(t) dt \end{aligned} \quad (\text{A.4})$$

The Laplace transform of the approximating function may be found by substituting the linear function segments defined in equation (A.2) into equation (A.4). As these functions are only defined for $t \leq T_N$, the shape of the function $f_{N+1}(t)$ must be assumed.

Assuming the function is constant for all times greater than T_N , that is $f_{N+1}(t) = F_N$, the Laplace transform for the piecewise linear function approximation from equation (A.4) becomes

$$F(s) = F_0 \frac{e^{-sT_0}}{s} + \frac{1}{s^2} \sum_{k=1}^N \dot{F}_k (e^{-sT_{k-1}} - e^{-sT_k}) \quad (\text{A.5})$$

Two other common treatments for the function extrapolation are to assume the function has a zero value for all times greater than T_N , or that the slope of the function is constant and equal to the slope of the last segment for all times greater than T_N . The resulting transform equations are given in equations (A.6) and (A.7) for the zero value and the constant slope assumptions respectively.

$$F(s) = F_0 \frac{e^{-sT_0}}{s} + \frac{1}{s^2} \left[\sum_{k=1}^N \dot{F}_k (e^{-sT_{k-1}} - e^{-sT_k}) \right] - F_N \frac{e^{-sT_N}}{s} \quad (\text{A.6})$$

$$F(s) = F_0 \frac{e^{-sT_0}}{s} + \frac{1}{s^2} \left[\sum_{k=1}^N \dot{F}_k (e^{-sT_{k-1}} - e^{-sT_k}) \right] + \dot{F}_N \frac{e^{-sT_N}}{s^2} \quad (\text{A.7})$$

Having obtained the Laplace transform of the flux function from one of the equations above, the solution for the concentration gradient in Laplace space may be found from equation (4.43). To obtain the solution in terms of time, the Laplace domain solution must be inverted numerically.

A review of methods for numerical inversion of Laplace transforms is given by Davies and Martin (1979). Several methods provide high levels of accuracy over a wide range of test functions, although no single method gave optimum results for all purposes. As a compromise between ease of implementation and accuracy, the algorithm presented

by Stehfest (1970) is used here. The applicability of this algorithm for transforming the boundary integral with various flux functions is discussed in Section 4.5, where results for the time domain and Laplace domain formulations are compared.

For a given time t , one concentration value ρ_i is generated from N values of concentration in Laplace space $\bar{\rho}_i(s_j)$, $j = 1, N$, according to the following formula:

$$\rho_i(t) = \frac{\ln 2}{t} \sum_{j=1}^N V_j \bar{\rho}_i\left(j \frac{\ln 2}{t}\right) \quad (\text{A.8})$$

where the weighting function V_j is calculated from

$$V_j = (-1)^{(N/2)+j} \sum_{k=(j+1)/2}^{\min(j, N/2)} \frac{k^{N/2} (2k)!}{(N/2 - k)! k! (k-1)! (j-k)! (2k-j)!} \quad (\text{A.9})$$

The number of terms N used in the expansion must be even, and the accuracy of the algorithm increases with increasing N . The values of the weighting function for several values of N are shown below in Table A.1. As can be seen from this table, machine precision limits are quickly reached, and a practical upper limit of $N = 8$ is found for single precision computing, $N = 16$ for double precision.

To generate one value of concentration at point x and time t , eight values of $\bar{\rho}_i(s_j)$ are calculated from equation (4.43), with $s_j = j \ln 2 / t$. These values are then summed according to equation (A.8), with the appropriate weighting functions given by equation (A.9), to give the desired value $\rho_i(t)$.

A.2. SOLUTION OF THE CONCENTRATION DIFFUSION EQUATION IN TWO DIMENSIONS

The boundary integral equations given in equation (4.18) for the time domain, and equation (4.19) for the Laplace domain may be used for problems in one, two, or three dimensions. The procedure for using these equations in two and three dimensions follows

Table A.1: Stehfest Algorithm Weighting Coefficients

j	Number of Coefficients			
	4	8	12	16
1	-2.0000000	-0.3333333	-0.016666666666667	-0.0003968253968254
2	26.0000000	48.3333300	16.01666666666670	2.133730158730160
3	-48.0000000	-906.0000000	-1247.000000000000	-551.0166666666670
4	24.0000000	5464.6670000	27554.33333333330	33500.16111111110
5		-14376.6700000	-263280.8333333330	-812665.1111111110
6		18730.0000000	1324138.700000000	10076183.76666670
7		-11946.6700000	-3891705.533333330	-73241382.97777780
8		2986.6670000	7053286.333333330	339059632.0730160
9			-8005336.500000000	-1052539536.278570
10			5552830.500000000	2259013328.583330
11			-2155507.200000000	-3399701984.433330
12			359251.2000000000	3582450461.700000
13				-2591494081.366670
14				1227049828.766670
15				-342734555.4285710
16				42841819.42857140

the same steps as those outlined in the previous section for the one-dimensional problem.

Application to a two-dimensional problem is shown below.

The diffusion equation will be solved for a rectangular region of dimensions x_e by y_e , again with the molar fluxes of component i across the block boundaries given as general functions of time. A schematic of the problem geometry is given in Figure A.1, below.

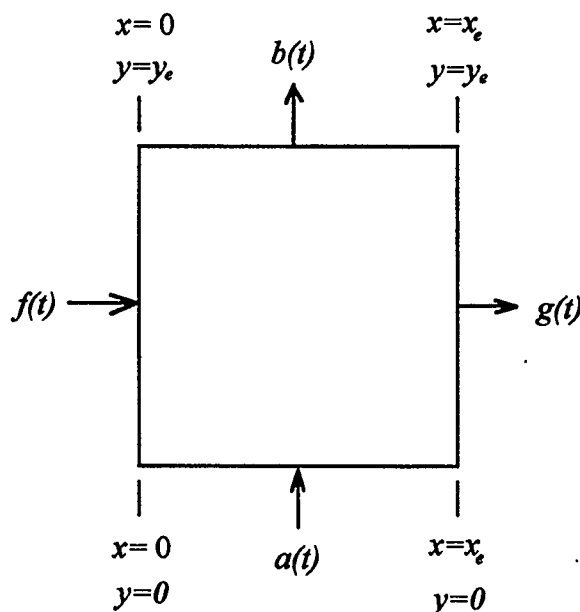


Figure A.1: Two Dimensional Problem Geometry

A.2.1. TIME DOMAIN SOLUTION

The diffusion equation given in equation (4.22) for the one dimensional problem can be extended to the two dimensional problem, assuming equal diffusivity in both directions, as

$$\frac{\partial \Delta \rho_i(x, y, t)}{\partial t} = D_i \left[\frac{\partial^2 \Delta \rho_i(x, y, t)}{\partial x^2} + \frac{\partial^2 \Delta \rho_i(x, y, t)}{\partial y^2} \right] \quad (\text{A.10})$$

The prescribed flux boundary conditions corresponding to the molar fluxes shown in Figure A.1 are written in the same form for each boundary as those given in equation (4.23) for the one dimensional problem. The zero initial condition again applies.

To solve this problem with the sources distributed over the boundaries of the region, equation (4.18) is written as:

$$\begin{aligned}
\Delta\rho_i(x,y,t) = & \int_0^t \left[\int_{y'=0}^{y'=y_e} f(\tau) G(x,y,y',t-\tau, x'=0) dy' + \int_{y'=0}^{y'=y_e} g(\tau) G(x,y,y',t-\tau, x'=x_e) dy' \right. \\
& \left. + \int_{x'=0}^{x'=x_e} a(\tau) G(x,y,y',t-\tau, y'=0) dx' + \int_{x'=0}^{x'=x_e} b(\tau) G(x,y,y',t-\tau, y'=y_e) dx' \right] d\tau
\end{aligned} \quad (A.11)$$

The source functions for this equation are obtained as described for the one-dimensional problem. Gringarten and Ramey (1973) give the source function for a two-dimensional rectangular region with prescribed flux at the boundaries as follows:

$$\begin{aligned}
G(x,x',y,y',t) = & \left\{ \frac{1}{x_e} \left[1 + 2 \sum_{n=1}^{\infty} \exp\left(\frac{-n^2 \pi^2 D_x t}{x_e^2}\right) \cos\left(\frac{n\pi x'}{x_e}\right) \cos\left(\frac{n\pi x}{x_e}\right) \right] \right\} \\
& \times \left\{ \frac{1}{y_e} \left[1 + 2 \sum_{n=1}^{\infty} \exp\left(\frac{-n^2 \pi^2 D_y t}{y_e^2}\right) \cos\left(\frac{n\pi y'}{y_e}\right) \cos\left(\frac{n\pi y}{y_e}\right) \right] \right\}
\end{aligned} \quad (A.12)$$

The final equation for the two-dimensional concentration profile may be obtained by substituting the appropriate source functions into the inner integrals in equation (A.11), and performing the integrations analytically. The component fluxes are assumed to be evenly distributed along the block boundaries (i.e. constant with respect to the space variable), thus they may be taken outside the spatial integrals. Performing these steps yields an equation which is simply the summation of two orthogonal one-dimensional solutions. The two-dimensional concentration profile equation may be written as:

$$\begin{aligned}
\Delta\rho_i(x,y,t) = & \int_0^t \left[f(\tau) G(x, x'=0, t-\tau) + g(\tau) G(x, x'=x_e, t-\tau) \right. \\
& \left. + a(\tau) G(y, y'=0, t-\tau) + b(\tau) G(y, y'=y_e, t-\tau) \right] d\tau
\end{aligned} \quad (A.13)$$

and the source functions are the same as for the one-dimensional case, given in equations (4.36) and (4.37).

A.2.2. LAPLACE DOMAIN SOLUTION

The two-dimensional diffusion equation in the Laplace domain corresponding to the one dimensional case given in equation (4.25), again assuming equal diffusivity in both directions, may be written as:

$$\frac{\partial \Delta \bar{\rho}_i(x, y, s)}{\partial t} = D_i \left[\frac{\partial^2 \Delta \bar{\rho}_i(x, y, s)}{\partial x^2} + \frac{\partial^2 \Delta \bar{\rho}_i(x, y, s)}{\partial y^2} \right] \quad (\text{A.14})$$

Again, the prescribed flux boundary conditions corresponding to the molar fluxes shown in Figure A.1 are written in the same form for each boundary as those given in equation (4.26) for the one dimensional problem.

The Laplace space boundary integral form, equation (4.19), for this case may be written:

$$\begin{aligned} \Delta \bar{\rho}_i(x, y, s) = & \int_{y'=0}^{y'=y_*} \bar{f}(s) \bar{G}(x, y, y', s; x' = 0) dy' + \int_{y'=0}^{y'=y_*} \bar{g}(s) \bar{G}(x, y, y', s; x' = x_*) dy' \\ & + \int_{x'=0}^{x'=x_*} \bar{a}(s) \bar{G}(x, y, y', s; y' = 0) dx' + \int_{x'=0}^{x'=x_*} \bar{b}(s) \bar{G}(x, y, y', s; y' = y_*) dx' \end{aligned} \quad (\text{A.15})$$

The source functions for this equation are obtained as described for the one-dimensional problem. van Kruijsdijk (1988) gives the Laplace space source function for a two-dimensional rectangular region with prescribed flux at the boundaries as follows:

$$\begin{aligned}
\bar{G}(x, y, x', y', s) = \frac{1}{2D_i x_e} \left\{ \frac{1}{\sqrt{s/D_i}} \left[\frac{2 \cosh[(y - y')\sqrt{s/D_i}]}{\exp(2y_e \sqrt{s/D_i}) - 1} + \exp[-|y - y'|\sqrt{s/D_i}] \right] \right. \\
+ \frac{2 \cosh[(y + y')\sqrt{s/D_i}]}{\exp(2y_e \sqrt{s/D_i}) - 1} + \exp[-|y + y'|\sqrt{s/D_i}] \left. + \sum_{n=1}^{\infty} 2 \frac{\cos(n\pi x/x_e) \cos(n\pi x'/x_e)}{\sqrt{s/D_i + (\pi n/x_e)^2}} \right. \\
\times \left[\frac{2 \cosh[(y - y')\sqrt{s/D_i + (\pi n/x_e)^2}]}{\exp(2y_e \sqrt{s/D_i + (\pi n/x_e)^2}) - 1} + \exp[-|y - y'|\sqrt{s/D_i + (\pi n/x_e)^2}] \right. \\
\left. + \frac{2 \cosh[(y + y')\sqrt{s/D_i + (\pi n/x_e)^2}]}{\exp(2y_e \sqrt{s/D_i + (\pi n/x_e)^2}) - 1} + \exp[-|y + y'|\sqrt{s/D_i + (\pi n/x_e)^2}] \right] \left. \right\} \quad (A.16)
\end{aligned}$$

As for the time domain solution, the final equation for the two-dimensional concentration profile in the Laplace domain, obtained by substituting the appropriate source functions into equation (A.15), is simply the summation of two orthogonal one-dimensional solutions. The two-dimensional concentration profile equation may be written as:

$$\begin{aligned}
\Delta \bar{\rho}_i(x, y, s) = \bar{f}(s) \bar{G}(x, x' = 0, s) + \bar{g}(s) \bar{G}(x, x' = x_e, s) \\
+ \bar{a}(s) \bar{G}(y, y' = 0, s) + \bar{b}(s) \bar{G}(y, y' = y_e, s) \quad (A.17)
\end{aligned}$$

with the source functions given by equations (4.44) and (4.45).

Extending this analysis to three-dimensional rectangular grid blocks, the concentration distribution equations may be written directly as the summation of three orthogonal one-dimensional solutions.

A.3. TIME DOMAIN/LAPLACE DOMAIN SOLUTION EVALUATION

From the development of the model equations shown in the previous sections, it can be seen that the two main advantages inherent in the Laplace space solution of the diffusion equation are: removal of the time integral in the boundary integral formulation,

equation (4.18), and the elimination of the infinite summation terms in the source functions, e.g. equation (4.34). The obvious disadvantage of the method is that the Laplace space solution must be inverted numerically to obtain the time domain solution. In order to use the Laplace domain solution with confidence, the applicability of the Stehfest Algorithm for the numerical inversion of the Laplace space concentration profiles must be verified.

In this section, results of the time domain solution procedure and the Laplace domain solution procedure are compared for five different flux functions. As the solutions for the two and three dimensional problems are simply obtained by superposition of the one dimensional solutions, the method will be validated for the one dimensional case only.

As discussed earlier, the flux functions must be extrapolated from the last known time value to infinity in order to use the Piecewise Linear Approximation (PLA) for the Laplace transform. Two extrapolation techniques were found to give good results: the constant value extrapolation, and the constant slope extrapolation. Results obtained using both of these methods are examined in this section.

A.3.1. RESULTS OF CONCENTRATION PROFILE CALCULATIONS

For the five cases studied, a component flux is defined for one end of the one dimensional grid block, at $x = 0$, while the other end at $x = x_e$ is considered impermeable. The concentration profile in the time domain is given by equation (4.35), with the source functions given by equations (4.36) and (4.37). The concentration profile in Laplace space is given by equation (4.43), with the source functions given by equations (4.44) and (4.45).

The concentration profile solutions are given in terms of the following dimensionless units:

$$t_D = \frac{D_i t}{x_e^2}, \quad x_D = \frac{x}{x_e}, \quad C_D = \frac{\rho_i(x, t)}{\rho_i^o}, \quad f_D(t_D) = \frac{f(t)x_e}{D_i \rho_i^o} \quad (\text{A.18})$$

The simplest case is that of a constant flux function:

$$f_D(t_D) = 1 \quad (\text{A.19})$$

As both the flux and the slope of the flux function are constant, both extrapolation methods for the Piecewise Linear Approximation yield the same results. Another consequence of the constant slope flux function is that the PLA will yield the exact Laplace transform of the flux function, thus any discrepancies in the solution profiles will be due to the Stehfest algorithm. The concentration profiles calculated using the time domain and Laplace domain solution techniques for this case are shown in Figure A.2 for

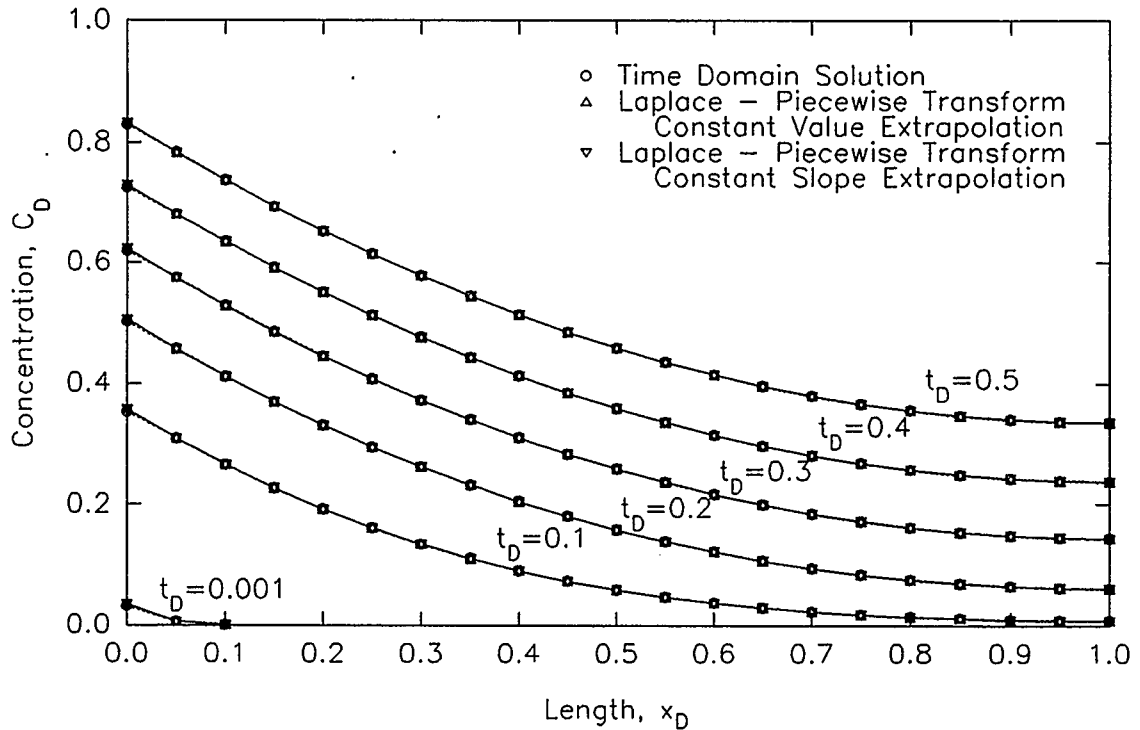


Figure A.2: Concentration Profiles - Constant Flux Function

several values of dimensionless time. As seen in this figure, the concentration profiles are virtually indistinguishable.

The next case studied is the ramp flux function with constant slope:

$$f_D(t_D) = t_D \quad (\text{A.20})$$

The calculated concentration profiles for this case are shown in Figure A.3. As expected, the Laplace domain solution with the constant slope extrapolation matches the time domain solution more closely than with the constant value extrapolation. Again, the PLA with the constant slope extrapolation will yield the exact Laplace transform of the flux function; the small variation in the solutions with this extrapolation method are due to the Stehfest algorithm. The somewhat larger errors associated with the constant value extrapolation are due to the combined effects of the extrapolation method and the inversion algorithm.

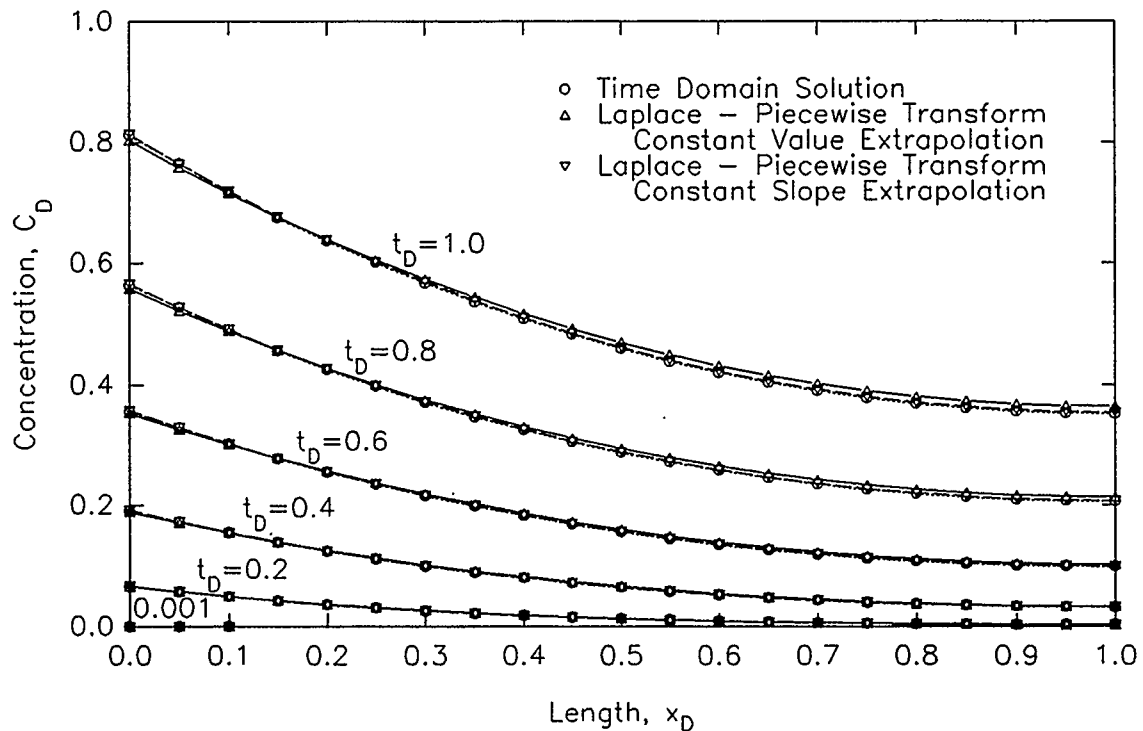


Figure A.3: Concentration Profiles - Ramp Flux Function

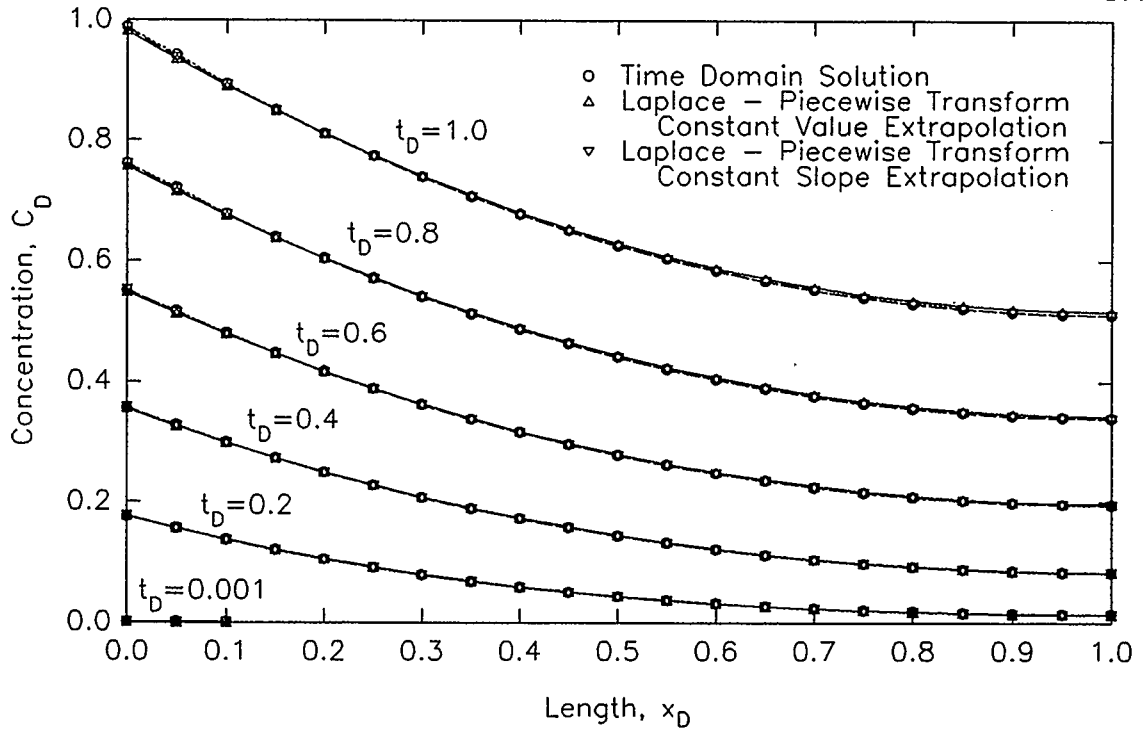


Figure A.4: Concentration Profiles - Square Root Flux Function

The third function tested is a square root form:

$$f_D(t_D) = \sqrt{t_D} \quad (\text{A.21})$$

In this case, the results of the Laplace domain solutions depend on the number of points used in the Piecewise Linear Approximation. In order to reduce the errors introduced by the PLA, the flux function must be approximated by a sufficiently large number of line segments. For times up to $t_D = 1$, it was found that the flux function could be adequately approximated with 25 points in the PLA. This value was used to generate the concentration profiles shown in Figure A.4. Again, the Laplace domain solution with the constant slope extrapolation is found to agree more closely with the time domain solution than the constant value extrapolation method.

Stehfest (1970) indicates that the Laplace inversion algorithm is not expected to give accurate results for functions with discontinuities or oscillations in the vicinity of the time for which the value of the function is desired. The effect of discontinuous or oscillatory flux functions on the accuracy of the diffusion equation solutions are examined next.

The discontinuous function chosen is a single step function. Roumboutsos (1988) has shown that the Piecewise Linear Approximation and the Stehfest algorithm may be used with functions of this type, provided the step is smoothed in some manner. Allowance for defining the step function with a finite slope is made here. The flux function is defined as:

$$f_D(t_D) = \begin{cases} q & 0 \leq t_D \leq t_{D_1}^* \\ q - \frac{t_D - t_{D_1}^*}{t_{D_1} \tan \delta} & t_{D_1}^* \leq t_D \leq t_{D_2}^* \\ 0 & t_{D_2}^* \leq t_D \end{cases} \quad (A.22)$$

$$t_{D_1}^* = t_{D_1} [1 - (q/2) \tan \delta]$$

$$t_{D_2}^* = t_{D_1} [1 + (q/2) \tan \delta]$$

In this case, we let $q = 1$ and $t_{D_1} = 1$. The amount of smoothing of the function depends on the value chosen for δ ; a value of $\delta = 0^\circ$ gives the step function with no smoothing, while a value of $\delta = 45^\circ$ would give a ramp function with constant slope. Values of $\delta = 0.1^\circ$, $\delta = 1^\circ$ and $\delta = 5^\circ$ are tested here.

For the Laplace domain solutions, the flux function is divided into three segments for the PLA corresponding to the three regions defined in equation (A.22). The time domain solutions are generated using the step function with no smoothing.

The effect of the slope chosen to smooth the step function is shown in Figures A.5 through A.7. In each of these figures, the calculated concentrations for five different

values of x_D are shown as a function of dimensionless time. These plots are shown in Figures A.5, A.6, and A.7 for δ values of 0.1° , 1° and 5° respectively. As the final segment in the PLA has a constant value, both extrapolation methods yield identical results; thus, only one Laplace solution curve and one time domain solution curve are shown in each plot.

From Figure A.5, it can be seen that the sampling method of the Stehfest algorithm causes oscillations in the solution with time when a small value of δ is used. For values of δ less than 0.1° , these oscillations are even larger. The effect of increasing δ is to decrease the amplitude of these oscillations; at $\delta = 5^\circ$ the oscillations are almost completely damped. Even without oscillations, the Stehfest algorithm gives erroneous results for the step function at times close to the step time, as shown in Figure A.7. Using a value of $\delta = 5^\circ$ to smooth the step function, however, the Stehfest algorithm may be used to approximate the time domain solution at times greater than $1t_D$ from the step time.

The calculated concentration profiles for five dimensionless times greater than $t_D = 1$ as functions of dimensionless length are shown in Figure A.8. As can be seen in these plots, the profiles in the transition period between $t_D = 1$ and $t_D = 2$ are not modeled accurately by the Laplace domain solution, however it does provide a good approximation to the steady-state solution.

The final flux function studied is a sine form:

$$f_D(t_D) = \sin(2\pi t_D) \quad (\text{A.23})$$

Based on the results obtained for the other flux functions, the PLA with 30 points is used for the function approximation in this case. The calculated concentration profiles are shown in Figure A.9. The results through one half cycle time $t_D = 0.5$ show reasonable agreement between the Laplace domain and time domain solutions. After this time,

however, the errors in the Laplace solution continue to increase; after one full cycle time, the Laplace domain solution fails to even follow the trends exhibited by the time domain solution.

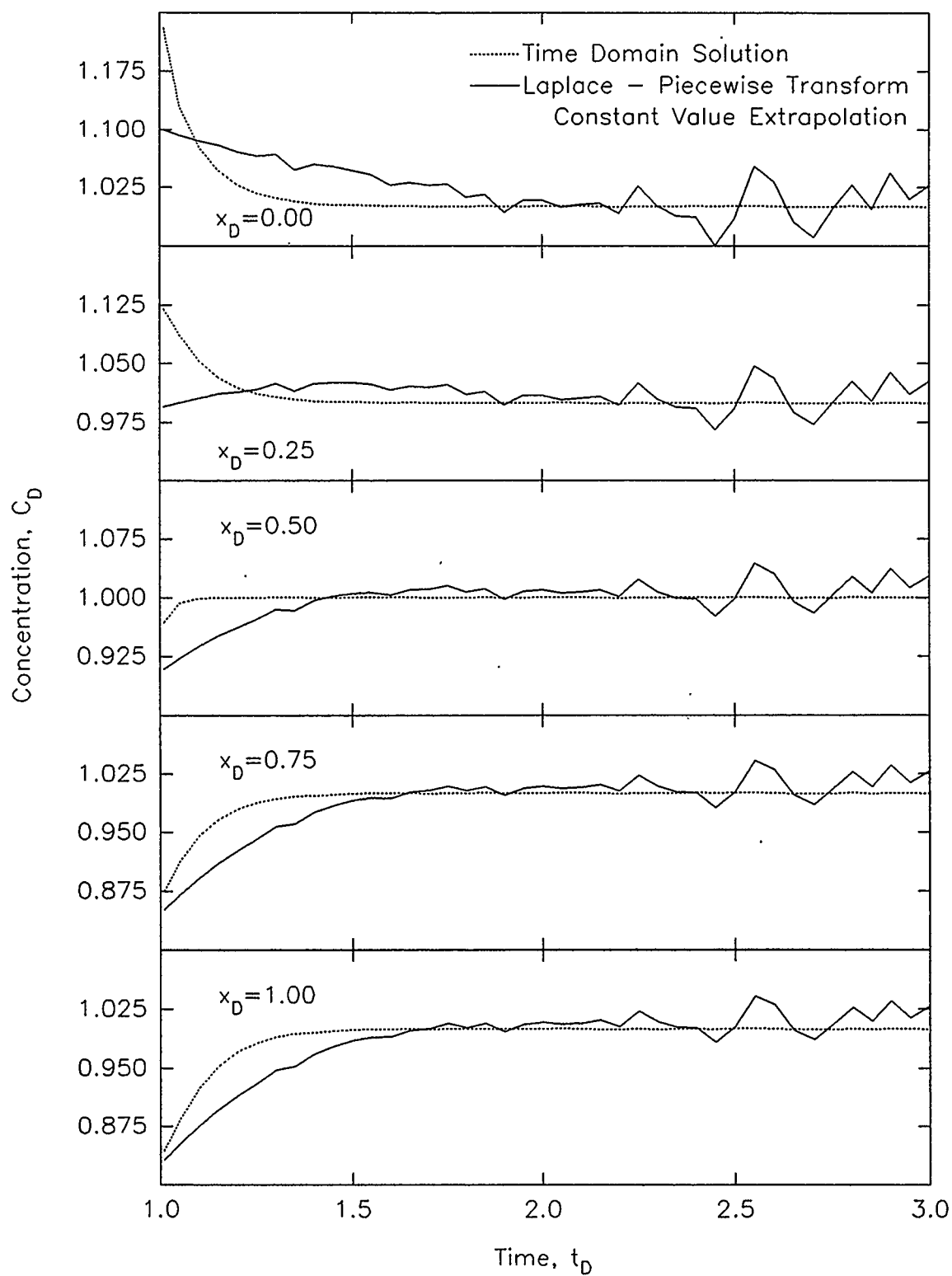


Figure A.5: Concentration Variation with Time - Step Flux Function ($\delta = 0.1^\circ$)

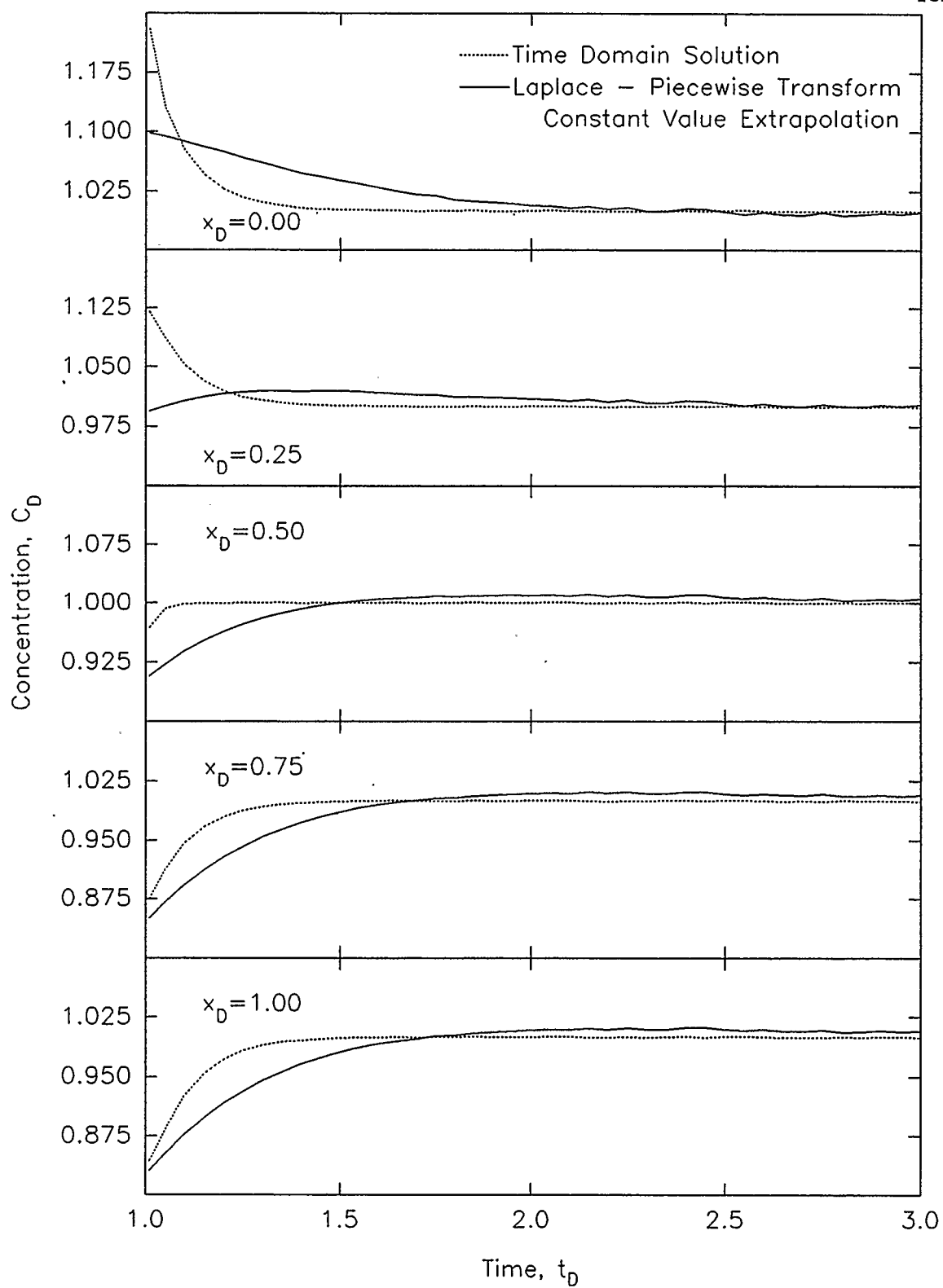


Figure A.6: Concentration Variation with Time - Step Flux Function ($\delta = 1.0^\circ$)

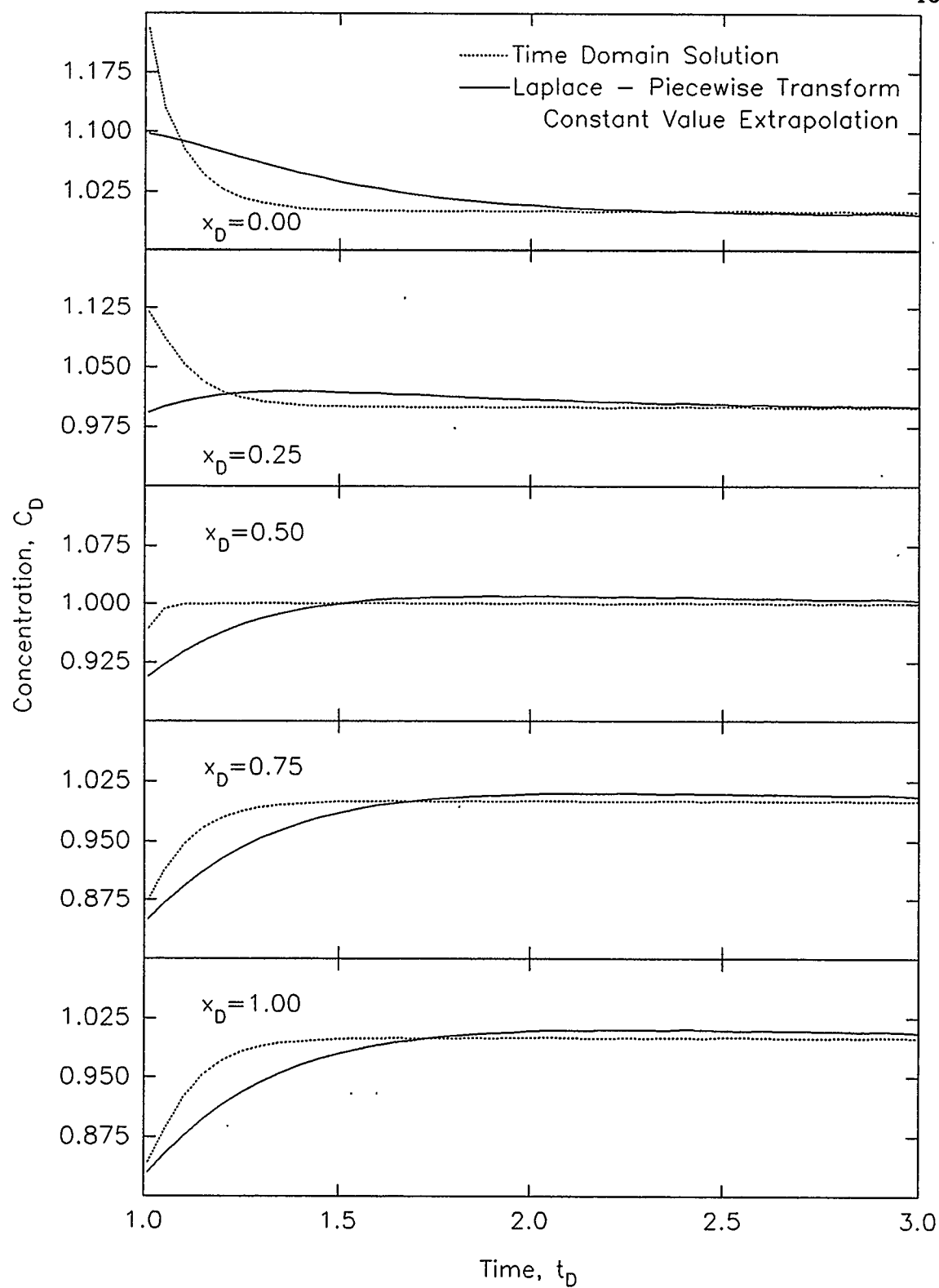


Figure A.7: Concentration Variation with Time - Step Flux Function ($\delta = 5.0^\circ$)

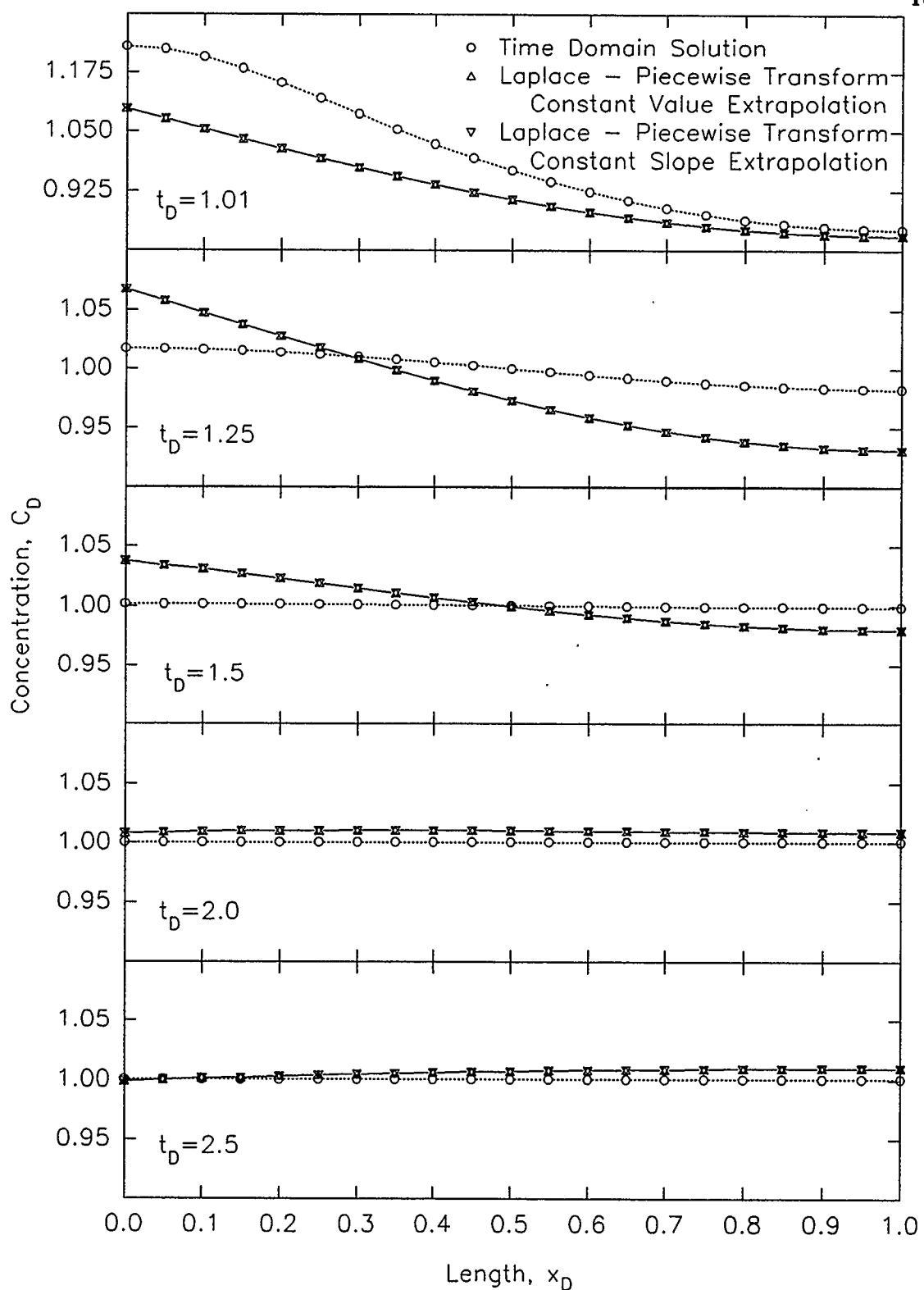


Figure A.8: Concentration Profiles - Step Flux Function ($\delta = 5.0^\circ$)

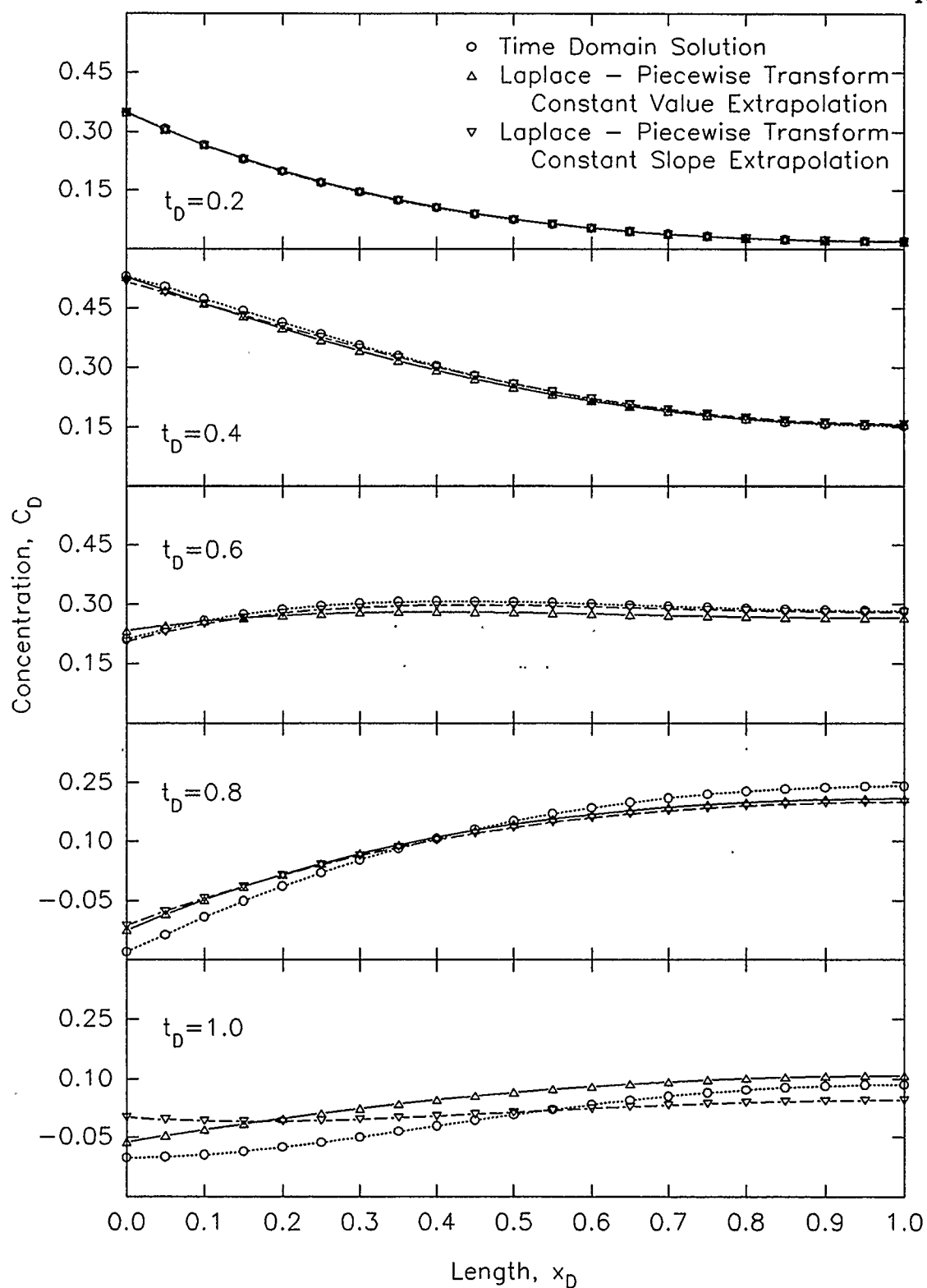


Figure A.9: Concentration Profiles - Sine Flux Function

A.3.2. SUMMARY OF LAPLACE AND TIME DOMAIN CALCULATIONS OF CONCENTRATION PROFILES

As noted earlier, the Laplace transform of the boundary integral equation was introduced to eliminate the numerical integration of the convolution integral in time, with the resulting formulation requiring numerical Laplace inversion instead. A comparison of the program execution times, for the generation of concentration profiles at six values of $t_D = 0.01, 0.1, 0.2, 0.3, 0.4,$ and 0.5 , using the time domain solution method and the Laplace domain solution methods with both extrapolation techniques are shown below in Table A.2. The execution times are for a DOS based PC with an 80386 processor and an 80387 math coprocessor.

Table A.2: Execution Times for Concentration Profile Generation

Solution Method	Flux Function				
	Constant	Ramp	Square Root	Step	Sine
Time Domain	4:49.08	4:50.45	4:37.21	4:13.15	5:25.22
Laplace Domain (Constant Value)	2.47	2.58	3.46	3.85	3.90
Laplace Domain (Constant Slope)	2.53	2.58	3.58	3.90	4.01

The execution times reflect the difficulty of performing numerical integration of the convolution integral with the infinite sum present in the source function. A standard Romberg integration routine is used for the evaluation of the convolution integral (Press et al.; 1986). At the small values of dimensionless time used in these calculations, the infinite sum requires a large number of terms to converge; the repeated evaluation of these sums in the numerical integration scheme uses considerable computation time. For larger values of t_D , the sums converge in just a few terms, resulting in much faster computation times. The Laplace inversion technique performs at the same speed regardless of the value of t_D .

It can be concluded that the Laplace domain solution method will proceed more quickly than the time domain solution, with the magnitude of the computation savings depending on the value of time for which a solution is desired.

The Laplace domain solution techniques may be used with reasonable accuracy for flux functions approximating any of the functions studied in this comparison except for oscillatory functions. The appearance of discontinuities in the flux function must be examined to determine if the desired value of concentration is at a point in time removed far enough from the discontinuity to allow solution with the step smoothing procedures described here.

A.4. FLUX EVALUATION WITH THE TIME DOMAIN AND LAPLACE DOMAIN SOLUTIONS

For both solution methods, the final step in obtaining the concentration profile is a numerical one: for the time domain solution it is a numerical integration, for the Laplace domain it is the numerical Laplace inversion. If the gradient of a profile calculated in the domain is required, the Laplace space expression may be differentiated analytically and this result inverted numerically. Similarly, the Laplace space profile expression may be integrated to determine the number of moles present in a given region, and again the resulting expression can be inverted numerically.