Adaptive-Implicit Method in Thermal Simulation

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Summary. An adaptive-implicit method (AIM) for thermal simulation that provides different degrees of implicitness in various gridblocks is discussed. A special treatment of flow terms during appearance or disappearance of any particular phase is critical. This treatment creates a more stable Jacobian matrix, especially in cases where an implicit block is downstream of an explicit neighbor. The maximum eigenvalue of a local amplification matrix, which is related to a dimensionless front velocity, determines the switching between implicit and explicit treatment. The switching, which is automatic and problem-independent, is superior to classical threshold switching based on the magnitude of changes of key reservoir variables. Results from the simulation of several thermal recovery processes are presented. The saving in computer time over a fully implicit method ranges from 34 to 62%. The maximum savings can be achieved in the simulation of large field-scale problems in which the fronts are moving fairly slowly.

Introduction

In early reservoir simulation models, the flow terms in the difference equations were handled explicitly. This posed some restrictions on timestep size because of numerical instability, especially in cases with extensive changes of key reservoir variables over a timestep. As reservoir simulation technology progressed, an emphasis was placed on implicit time-differencing methods. This approach reduced numerical instability, but larger time-truncation errors were introduced. In addition, computational cost and storage requirements are higher for the implicit method.

Usually, only a small portion of a reservoir experiences rapid changes in pressure, saturation, and temperature and must be treated implicitly. Thomas and Thurnau[1] proposed an AIM that provides different degrees of implicitness in various gridblocks. The switching between explicit and implicit treatments was based on pressure and saturation changes during an iteration. These changes were compared with specified threshold values. Several authors subsequently implemented this idea of varied implicitness in black-oil,[2-4] compositional,[5,6] and thermal[7,8] simulators with some dissimilarities in the handling of the explicit variables and in the switching between explicit and implicit modes.

More particularly, in a steamflood application of the adaptive-implicit technique, Tan[7] compared the performance of an AIM (similar to that of Thomas and Thurnau[1]) and an inexact adaptive Newtonian method (AIN) with different kinds of switching criteria on the problems of the Fourth SPE Comparative Solution Project. The implementation of AIM was unsuccessful [CPU time was higher than for fully implicit method (FIM) or non-convergence]. With the AIN method, savings from 5 to 28% were achieved.

Fung *et al.*[4] described a new switching criterion based on the numerical stability of a local amplification matrix. It is problem-independent and provides the possibility of backward switching (implicit to explicit), which is not feasible with the classical threshold switching criterion.

The implementation of an AIM in a multicomponent, multiphase thermal simulator is discussed in this paper. The switching criterion is similar to that of Fung *et al.*[4] Results are presented for both steam and combustion problems.

Model Description

The basic equations used in thermal simulation consist of mass- and energy-conservation equations. The mass conservation is expressed in terms of components; the energy equation is the total energy balance. The equations can be written as follows.

Mass balance for Component ic in n_P phases:

$$\underbrace{\sum_{P=1}^{n_P} \Delta[T\rho_P\lambda_P x_{P,ic}(\Delta p+\Delta P_{cP}-\gamma_P\Delta z)]}_{\text{flow term}}$$

$$= \underbrace{\frac{V}{\Delta t}\Delta_t \sum_{P=1}^{n_P} \phi\rho_P S_P x_{P,ic}}_{\text{accumulation}} + \underbrace{\sum_{irx=1}^{n_{rx}} s_{irx,ic}}_{\text{reaction}} + \underbrace{q_{m,ic}}_{\substack{\text{injection/}\\ \text{production}}} .$$

Total energy balance:

$$\underbrace{\sum_{P=1}^{n_P} \Delta[T\rho_P\lambda_P H_P(\Delta p+\Delta P_{cP}-\gamma_P\Delta z)]}_{\text{flow term}} + \underbrace{\Delta(T_{kh}\Delta T)}_{\substack{\text{thermal}\\ \text{conduction}}}$$

$$= \underbrace{\frac{V}{\Delta t}\Delta_t\left[\sum_{P=1}^{n_P} \phi\rho_P S_P E_P\right]}_{\text{fluid accumulation}} + \underbrace{(1-\phi)(\rho c_p)_r(T-T_r)}_{\text{rock accumulation}}$$

$$+ \underbrace{\sum_{irx=1}^{n_{rx}} s_{u,irx}}_{\text{reaction}} + \underbrace{q_E}_{\substack{\text{injection/}\\ \text{production}}} + \underbrace{Q_{\text{loss}}}_{\text{heat loss}} + \underbrace{Q_E}_{\substack{\text{external}\\ \text{heaters}}} .$$

In addition to the conservation equations, a saturation or gas mole fraction constraint equation exists that may be solved simultaneously with the reservoir flow equations.

In an implicit block, all terms in the conservation equations are evaluated at the latest timestep and iteration level. Derivatives with respect to all primary variables are included in the Jacobian matrix.

Treatment of explicit blocks is more complicated. The terms on the right side of the mass- and energy-balance equations (accumulation, reaction, injection, production, heat loss, and external heaters) are fully implicit. Flow and thermal conductivity terms are on the n level (previous timestep) during timesteps without phase change; fully implicit pressure derivatives are retained. As soon as a phase appears or disappears in the reservoir, the flow and conductivity terms are updated at that Newton iteration and kept on this iteration level for the rest of the timestep. However, the block is still handled explicitly; i.e., only derivatives with respect to pressure are included in the Jacobian matrix. This update is crucial to thermal problems because it creates a more stable Jacobian matrix, especially in cases where an implicit block is downstream of an explicit neighbor.

The Jacobian matrix is built columnwise into a packed array and solved by the adaptive implicit matrix solver (AIMSOL).[9] AIMSOL is a general sparse solver that uses incomplete Gaussian elimination as a preconditioning step to ORTHOMIN acceleration. The incomplete factorization is carried out in a block equation sense, implying that the symbolic factorization need be computed only when the block nonzero structure of the Jacobian matrix changes (e.g., well changes) and is independent of the implicitness level. A preprocessing step eliminates an arbitrarily specified subset of equations (well

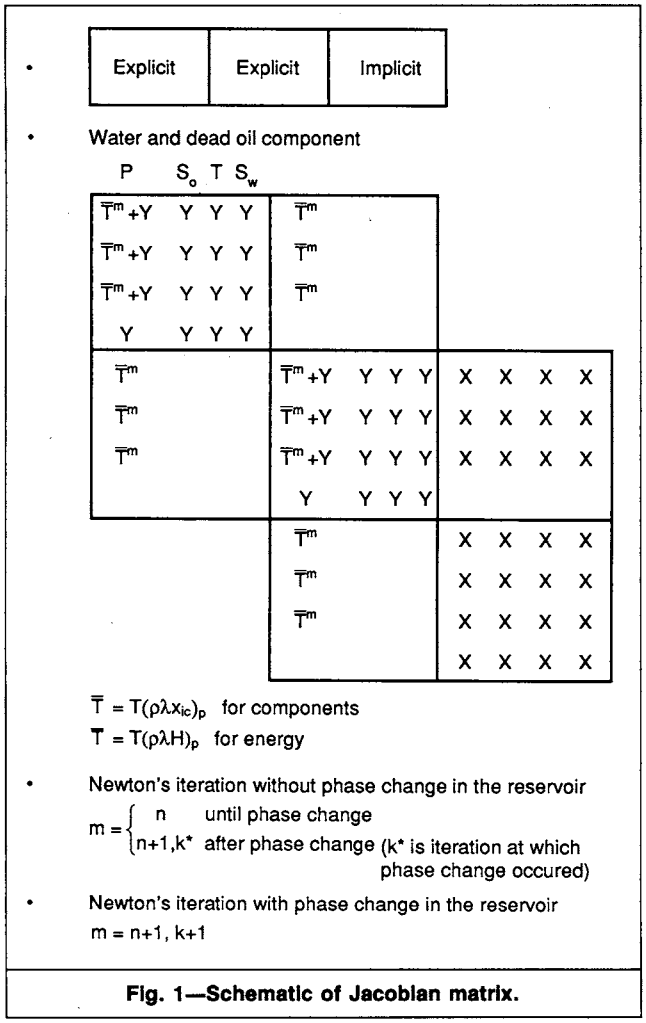

Fig. 1—Schematic of Jacobian matrix.

equations, constraint equations, and equations for explicit variables). **Fig. 1** shows an example of a Jacobian matrix structure and the treatment of flow and thermal conduction terms.

Implicit treatment is forced on gridblocks with external source/sink terms, such as wells and heaters.

Switching Criteria

The "implicitness" or percentage of blocks treated implicitly is adaptive because a gridblock can switch modes on the basis of local conditions at that point in time.

Stability Switching Criterion. The stability switching criterion is based on the work of Fung *et al.*[4] and involves the calculation of the maximum eigenvalue of a local amplification matrix

$$\mathbf{A}_{il}=\left[\frac{\partial f_j^{n+1,k+1}}{\partial v_i^{n+1,k+1}}\right]^{-1}\left[\frac{\partial f_j^{n+1,k+1}}{\partial v_\ell^{n}}\right],$$

which is a product of two matrices; the subscript j runs over all equations, and the subscripts i and ℓ over all primary variables.

The stability condition with respect to transmissibilities for an explicit method states that a moving front may not advance more than one gridblock per timestep.[10] To satisfy this condition on the local level, the norm of Matrix **A** must be ≤ 0. The eigenvalue is evaluated by a power method,[11] which calculates only the largest-magnitude eigenvalue. This poses some problems, especially in processes with multiple moving fronts. Therefore, the n-level accumulation term is handled in such a way that the maximum absolute value found by the power method will satisfy the stability condition. When the maximum eigenvalue for any particular gridblock is greater than two, numerical instability requires that the block must be treated implicitly. Fung *et al.*[4] did not include the n-level accumulation term in evaluation of the amplification matrix (see Eq. A-2h) and therefore set the stability limit as $|\alpha_{max}| \leq 1$. This treatment proved to be less successful than that implemented here. Physically, the maximum eigenvalue relates to the velocity of a predominant front. The relationship between α_{max} and the velocity of a moving front is shown in the Appendix for a geothermal problem (hot-water injection into a water reservoir). The same is true for the classic Buckley-Leverett problem.

The stability is checked only in the vicinity of an implicit front at the beginning of each timestep and during the appearance or disappearance of phases. Sometimes gridblocks behind the slowest-moving front do not need to be treated implicitly. Therefore, implicit blocks are checked every specified number of timesteps or at each well change for potential stability as explicit blocks. When the corresponding maximum eigenvalue is <1.3, the block is switched back to explicit mode. Use of a lower value (i.e., 1.3 as opposed to 2.0) avoids a large amount of marginal switching. Experience has shown that use of a higher value causes more blocks to switch back to explicit treatment, which often causes numerical instability or oscillation in switching. This backward switching proved to be very useful in the simulation of processes with stable fronts.

Threshold Switching Criterion. In threshold switching, a certain value is selected for each primary variable to which the change of primary variables over a Newtonian iteration is compared. When the change is greater than the chosen threshold value, the explicit block is switched to implicit mode. It is problem-dependent and an implicit block cannot switch back to an explicit treatment. Usually, the choice of threshold switching criterion is not very sensitive in steam problems. In combustion processes, however, the sensitivity of run performance to threshold values is fairly critical.

TABLE 1—SPE PROBLEM 2A

	First-Degree ILU Factorization	Gaussian Elimination
AIM		
Number of timesteps	82	79
Number of iterations	461	439
CPU AIM/CPU FIM	0.91	0.53
FIM		
Number of timesteps	72	72
Number of iterations	370	408

Results

The AIM can handle a wide range of thermal problems. Results will be shown for cyclic steam injection, steamdrive, steam plus additives, and laboratory and field combustion. As is well known, the CPU savings of AIM depend on problem size and on the degree of incomplete LU (ILU) factorization of the sparse Jacobian matrix. Generally, the CPU work increases with higher degrees of ILU factorization for both AIM and FIM, but is much higher for FIM. For example, **Table 1** shows the ratio between CPU times for AIM and FIM for two extreme cases, first-degree ILU factorization and complete LU factorization.

Differences between predicted reservoir performances obtained with AIM and FIM are minimal. **Fig. 2** shows oil production rates for a far producer for SPE Problem 3A.

Six thermal simulation problems were used to illustrate the performance of AIM. Apollo DN3000 and DN10000 workstations were used in computations. The first three examples are from the Fourth SPE Comparative Solution Project.[12]

Example 1. Cyclic steam injection into a dead-oil reservoir was simulated with a 2D radial cross-sectional 13×4 grid. Three cycles consisting of 10 days steam injection, 7 days soak, and 348 days production were simulated. Initially the reservoir was treated explicitly except for the wellblocks. At the beginning of each subcycle, the implicit blocks were checked for a potential stability as explicit blocks and switched to explicit treatment if stable.

The importance of the flow-term updates for the explicit blocks during phase changes in the reservoir is demonstrated in this prob-

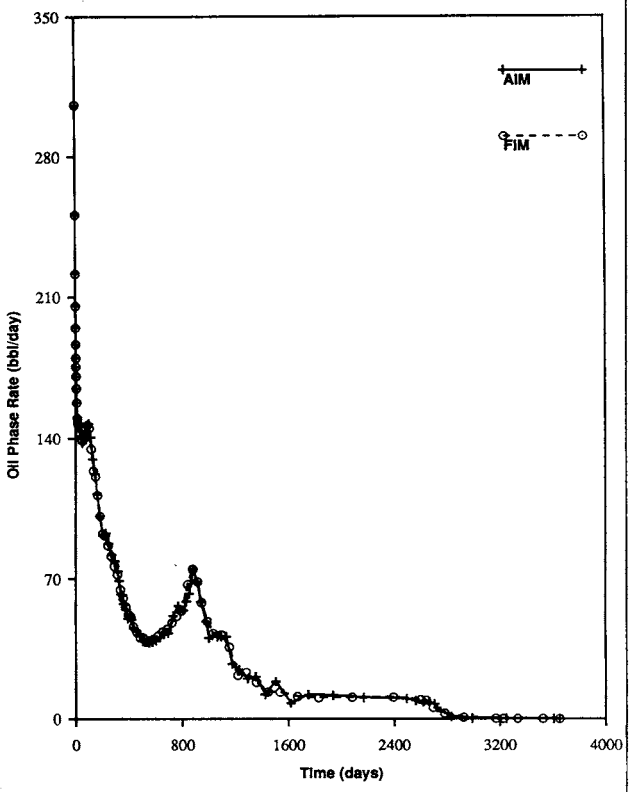

Fig. 2—SPE Problem 3 A: steam injection, oil phase rate vs. time.

lem. The injection and production are separated and it is very easy to establish the upstream direction. During the injection cycle, the upstream blocks are implicit and the performance of AIM without flowterm updates is not affected. As soon as the upstream direction switches during the production cycle (implicit block is downstream of an explicit neighbor), difficulties occur and the performance deteriorates. **Table 2** illustrates this behavior and the implemented AIM.

Example 2. Displacement of dead oil by steam in one-eighth of an inverted nine-spot pattern (9×5×4 Cartesian grid) is simulated. Nine-point discretization is used to avoid excessive grid-orientation effects.

In this case, as in most steam processes, the velocity of the moving steam front determines the switching between explicit and implicit treatments. As **Fig. 3** shows, the steam front either trails or coincides with the implicit front. The comparison of AIM and FIM performance is in Table 1.

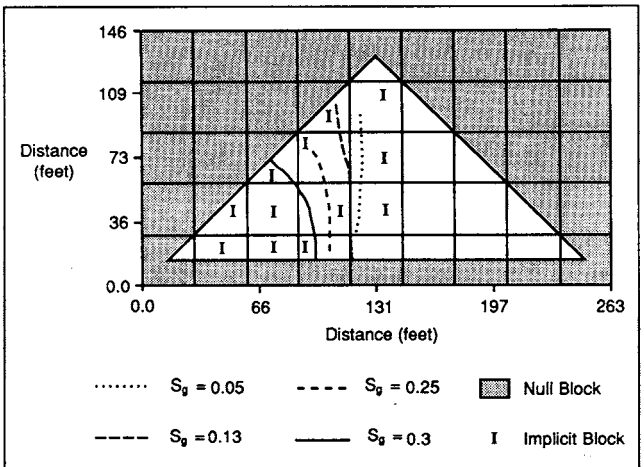

Fig. 3—SPE Problem 2A: steam injection, gas saturation and implicit front at 1,095 days.

TABLE 2—SPE PROBLEM 1A

	FIM	AIM	AIM*
End of first injection cycle, days	10.0	10.0	10.0
Number of timesteps	21	22	21
Number of iterations	102	109	97
End of first production cycle, days	365	365	365
Number of timesteps	35	40	40
Number of iterations	167	198	233
End of third production cycle, days	1,095	1,095	1,095
Number of timesteps	111	117	130
Number of iterations	506	553	699
CPU AIM/CPU FIM	—	0.56	0.75

*AIM without flow-term updates during phase changes.

Example 3. Steamdrive in the reservoir with the same configuration as in Example 2 is simulated with different fluids. The oil phase contained two volatile and one nonvolatile hydrocarbon components. Switching behavior was similar to that in Example 2 with 10% CPU savings (**Table 3**) when first-degree ILU factorization was used.

Example 4. Displacement of bitumen in a heterogeneous high-pressure laboratory physical simulator (8×16 radial cross-sectional grid) was simulated.[13] The wells were connected with a high-permeability, high-water-saturation communication path. A truncated injection strategy was chosen here relative to the actual experiment. Seven hours of steam injection was followed by 7 hours of steam and dual-additive (CO_2 and naphtha) injection.

In this example, the oil mobility is much smaller than in the previous problems. The oil viscosity depends strongly on temperature; therefore, the temperature front moving ahead of the steam front causes instability in the explicit blocks during the pure-steam injection cycle. During the additive injection, instability is a combined effect of CO_2 and naphtha in gas and liquid phases and temperature, as illustrated in **Fig. 4**. The CPU savings are fairly high (**Table 4**) because all effects initially are restricted to the neighborhood of the communication path.

Example 5. Forward wet combustion in an adiabatic vertical tube with three liquid hydrocarbon components and two noncondensable gases was matched.[14] The 0.69-in.-long tube was divided into 20 uniform gridblocks. Air was injected at the top of the tube for 2.88 minutes, followed by coinjection of water and air.

The moving fronts propagated through the tube fairly quickly, and all blocks had to be treated implicitly before the end of air-only injection. As expected, the CPU savings with the stability switching criterion was only 4%. This suggests that the high throughput associated with standard combustion-tube experiments tends to preclude the use of AIM.

Some difficulties were encountered with the threshold switching criterion. Switching from explicit to implicit treatment was not fast enough to respond to the oxygen mole fraction changes, which resulted in oxygen mass-balance problems throughout the run.

Example 6. Cyclic steam stimulation was simulated with coke deposition followed by several cycles of air, oxygen, and cold-water

TABLE 3—SPE PROBLEM 3A

	First-Degree ILU Factorization	
	FIM	AIM
Number of timesteps	78	87
Number of iterations	408	494
CPU AIM/CPU FIM	—	0.9

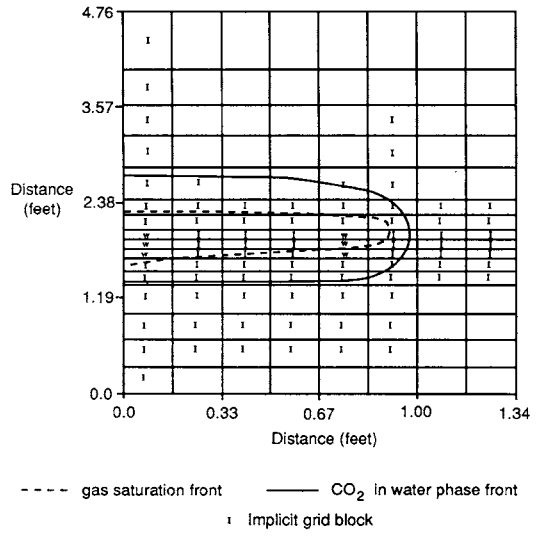

Fig. 4—Steam injection with dual additives after 7 hours of steam and 7 hours of steam and additives injection.

TABLE 4—STEAM INJECTION WITH DUAL ADDITIVES

	Gaussian Elimination	
	FIM	AIM
Number of timesteps	98	101
Number of iterations	397	389
CPU AIM/CPU FIM	—	0.39

TABLE 5—EXAMPLE NUMBER 6

	Second-Degree ILU Factorization	
	FIM	AIM
Cycling and coke deposition for 1,500 days		
Number of timesteps	729	723
Number of iterations	3,843	3,793
CPU AIM/CPU FIM	—	0.59
Air, oxygen, and cold-water injection for 995 days		
Number of timesteps	349	341
Number of iterations	2,449	2,579
CPU AIM/CPU FIM	—	0.67

injection.[15,16] Part of the repeated five-spot pattern was simulated. The formation fractured during the steam injection. Because the pressure is always handled implicitly in the AIM, the stability criterion did not respond to the reservoir fracturing. Therefore, additional switching criterion had to be applied to the fracture. Explicit blocks switched to implicit treatment as the fracture progressed. When the fracture healed during the production cycle, implicit blocks switched back to explicit mode.

During the 1,500 days of steam stimulation, the fracturing and steam front controlled the switching. The CPU time for the AIM with second-degree ILU factorization was 41% less than for the FIM. During the air, oxygen, and cold-water injection cycles, the CPU savings were 33% (**Table 5**). In this problem, the switching was caused mostly by the high-velocity gas front or the moving temperature front.

Conclusions

A robust, problem-independent switching criterion is an important tool in applying the AIM to a thermal simulator. Moreover, the treatment of explicit blocks is a significant factor in AIM performance. Updates of explicit flow terms with implicit pressure are necessary during phase changes. If flow-term updates are not done, CPU time increases and failure is possible. In a simulator with an iterative matrix solver, the CPU savings for the AIM will be affected by the degree of ILU factorization.

In steam processes, the switching is triggered either by the appearance of gas or by a moving temperature front in heavy-oil reservoirs. In combustion problems, the cause of switching is less clear because of multiple moving fronts that can change their relative positions during the process.

Nomenclature

a = matrix coefficient
$\mathbf{A}$ = local amplification matrix
c_p = molar heat capacity, Btu/(lbm mol-°F)
E = internal energy, Btu/lbm mol
$f_j^{n+1,k+1}$ = residual of jth conservation equation in $k+1$ Newtonian iteration of $n+1$ timestep
H = fluid enthalpy, Btu/lbm mol
k = permeability, md
n_c = number of components
n_P = number of phases
n_{rx} = number of reactions
p = pressure, psi
P_c = capillary pressure, psi
q_E = injection/production of energy, Btu/D
q_m = injection/production of mass, lbm mol/D
Q_E = energy sink/source from external heaters, Btu/D
Q_{loss} = heat loss to overburden and underburden, Btu/D
s = reaction component sink/source term, lbm mol/D
s_u = reaction heat sink/source term, Btu/D
S = saturation
t = time, days
T = transmissibility, ft^3
$\bar{T}$ = variable defined in Fig. 1
T_{kh} = thermal conductivity transmissibility, Btu/(D-°F)
T_r = reference temperature, °F
u_T = velocity, ft/D
$v_i^{n+1,k+1}$ = primary variable i in $k+1$ Newtonian iteration of $n+1$ timestep
v_ℓ^n = primary variable ℓ on n timestep level
V = gridblock volume, ft^3
x = mole fraction
X,Y = matrix entries not equal to 0
y = direction, ft
z = depth, ft
$\alpha_{\max}$ = maximum eigenvalue
λ = mobility kr/μ, psi^{-1}/D
ρ = molar density, lbm mol/ft^3
ϕ = porosity

Subscripts

g = gas phase
i = gridblock
ic = component
irx = reaction
k = Newton iteration
n = time level
o = oil
P = phase
r = rock
w = water

Superscripts

m = index defined in Fig. 1
$'$ = derivative

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Appendix—Relationship Between Maximum Eigenvalue and Moving Front Velocity

In the following derivation, the eigenvalue is shown to relate to the velocity of a moving front in the stability switching criterion. For simplicity, hot-water injection into a cold-water reservoir is considered. From fractional-flow theory, the velocity of a constant-temperature front is[17]

$$\left(\frac{dy}{dt}\right)_T = \frac{u_T \rho_w c_{pw}}{\phi \rho_w c_{pw} + (1-\phi)(\rho c_p)_r}. \quad \text{(A-1)}$$

The mass-water-conservation and total-energy-balance equations are considered. The heat-loss and sink/source term from external heaters, capillary pressure, and gravity are neglected. It is assumed that enthalpy and internal energy are functions of temperature only (with constant specific heats). If flow rates are high, we are able to neglect heat conduction. The pressure and temperature are primary variables.

The derivatives in the amplification Matrix **A** are

$$\frac{\partial f_w^{n+1,k+1}}{\partial p_i^{n+1}} = -(T\rho_w\lambda_w)_{i+\frac{1}{2}} - (T\rho_w\lambda_w)_{i-\frac{1}{2}}, \quad \text{(A-2a)}$$

$$\partial f_w^{n+1,k+1}/\partial p_i^n = 0, \quad \text{(A-2b)}$$

$$\partial f_w^{n+1,k+1}/\partial T_i^{n+1} = 0, \quad \text{(A-2c)}$$

$$\partial f_w^{n+1,k+1}/\partial T_i^n = 0, \quad \text{(A-2d)}$$

$$\frac{\partial f_E^{n+1,k+1}}{\partial p_i^{n+1}} = -(T\rho_w\lambda_w H_w)_{i+\frac{1}{2}} - (T\rho_w\lambda_w H_w)_{i-\frac{1}{2}}, \quad \text{(A-2e)}$$

$$\partial f_E^{n+1,k+1}/\partial p_i^n = 0, \quad \text{(A-2f)}$$

$$\frac{\partial f_E^{n+1,k+1}}{\partial T_i^{n+1}} = -\frac{V}{\Delta t}[\phi\rho_w E'_w + (1-\phi)(\rho c_p)_r]^{n+1}, \quad \text{(A-2g)}$$

and $$\frac{\partial f_E^{n+1,k+1}}{\partial T_i^n} = -(T\rho_w\lambda_w \Delta p H'_w)_{i+\frac{1}{2}} + \frac{V}{\Delta t} \times [\phi\rho_w E'_w + (1-\phi)(\rho c_p)_r]^n. \quad \text{(A-2h)}$$

Expressing the amplification Matrix **A** in terms of the above derivatives results in

$$\mathbf{A} \equiv \frac{-1}{D}\begin{bmatrix} \frac{\partial f_w^*}{\partial T_i^*}\frac{\partial f_E^*}{\partial p_i^n} - \frac{\partial f_w^*}{\partial p_i^n}\frac{\partial f_E^*}{\partial T_i^*}; & \frac{\partial f_w^*}{\partial T_i^*}\frac{\partial f_E^*}{\partial T_i^n} - \frac{\partial f_w^*}{\partial T_i^n}\frac{\partial f_E^*}{\partial T_i^*} \\ \frac{\partial f_E^*}{\partial p_i^*}\frac{\partial f_w^*}{\partial p_i^n} - \frac{\partial f_E^*}{\partial p_i^n}\frac{\partial f_w^*}{\partial p_i^*}; & \frac{\partial f_E^*}{\partial p_i^*}\frac{\partial f_w^*}{\partial T_i^n} - \frac{\partial f_E^*}{\partial T_i^n}\frac{\partial f_w^*}{\partial p_i^*} \end{bmatrix}, \quad \text{(A-3)}$$

where $*=n+1,k+1$ and $D=(\partial f_E^*/\partial T_i^*)(\partial f_w^*/\partial p_i^*)-(\partial f_E^*/\partial p_i^*)(\partial f_w^*/\partial T_i^*)$.

The eigenvalues, α, are calculated from a determinant of a matrix

$$\begin{bmatrix} a_{11}-\alpha & a_{12} \\ a_{21} & a_{22}-\alpha \end{bmatrix}:$$

$$\text{Det} = (a_{11}-\alpha)(a_{22}-\alpha) - a_{12}a_{21}$$

and $$\alpha_{1,2} = \frac{a_{22}+a_{11} \pm \sqrt{(a_{22}+a_{11})^2 - 4(a_{11}a_{22}-a_{12}a_{21})}}{2}. \quad \text{(A-4)}$$

Because $\partial f_w^{n+1,k+1}/\partial p_i^n$, $\partial f_w^{n+1,k+1}/\partial T_i^{n+1}$, $\partial f_w^{n+1,k+1}/\partial T_i^n$, and $\partial f_E^{n+1,k+1}/\partial p_i^n = 0$; a_{11}, a_{12}, and $a_{21} = 0$ and a_{22} reduces to $(\partial f_E^*/\partial T_i^n)/(\partial f_E^*/\partial T_i^*)$. Then, $\alpha_1 = 0$ and $\alpha_2 = a_{22}$.

Substituting the derivatives in α_2 results in

$$\alpha_2 = \frac{-(T\rho_w\lambda_w\Delta p H'_w)_{i+\frac{1}{2}} + (V/\Delta t)[\phi\rho_w E'_w + (1-\phi)(\rho c_p)_r]^n}{-(V/\Delta t)[\phi\rho_w E'_w + (1-\phi)(\rho c_p)_r]^{n+1}}$$

$$= \left(\frac{k\lambda_w \Delta p}{\Delta x}\right)\left\{\frac{\rho_w c_{pw}}{\phi\rho_w c_{pw} + (1-\phi)(\rho c_p)_r}\frac{\Delta t}{\Delta x} - \frac{[\phi\rho_w c_{pw} + (1-\phi)(\rho c_p)_r]^n}{[\phi\rho_w c_{pw} + (1-\phi)(\rho c_p)_r]^{n+1}}\right\}. \quad \text{(A-5)}$$

Thus, $$\alpha_2 = \frac{u_T\rho_w c_{pw}}{\phi\rho_w c_{pw} + (1-\phi)(\rho c_p)_r}\frac{\Delta t}{\Delta x} - 1 \quad \text{(A-6)}$$

because $u_T = k\lambda_w \Delta p/\Delta x$.

To satisfy the stability criterion for an explicit block,

$$\frac{u_T\rho_w c_{pw}}{\phi\rho_w c_{pw} + (1-\phi)(\rho c_p)_r}\frac{\Delta t}{\Delta x} \le 1, \quad \text{(A-7)}$$

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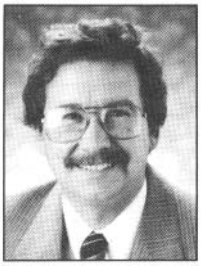
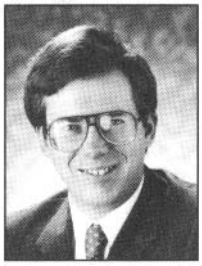

Coombe


Buchanan

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α_2 must be ≤ 0. The implemented $\bar{\alpha}_2$ is

$$\bar{\alpha}_2=\alpha_2+2\frac{[\phi\rho_w c_{pw}+(1-\phi)(\rho c_p)_r]^n}{[\phi\rho_w c_{pw}+(1-\phi)(\rho c_p)_r]^{n+1}}\leq 2. \quad \ldots\ldots\ldots \text{(A-8)}$$

In this way the stability region is symmetrical around zero.

SI Metric Conversion Factors

bbl	×	1.589 873	E−01	= m^3
ft	×	3.048*	E−01	= m
in.	×	2.54*	E+00	= cm

*Conversion factor is exact.

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Discussion of Adaptive-Implicit Method in Thermal Simulation

Noaman El-Khatib, SPE, King Saud U.

The energy balance in the model of Oballa *et al.* (Nov. 1990 *SPERE*, Pages 549–54) contains the heat of reaction explicitly as a source term. The inclusion of this term in the energy equation is wrong and violates the first law of thermodynamics. Because previously published thermal models also included such a term,[1-4] it is felt appropriate to clarify this point and present the correct form of the energy equation that should be used.

The energy balance in Oballa *et al.*'s paper included explicitly the term

$$\sum_{irx=1}^{n_{rx}} S_{u,irx},$$

where $S_{u,irx}$ represents the heat generated by the ith reaction and the summation is over the total number of reactions, n_{rx}. The heat generated by a chemical reaction may be expressed in terms of the reaction rate, k, and the heat of reaction ΔQ of a particular chemical reaction. Thus

$$S_{u,irx}=\Delta Q_{irx}k_{irx}. \quad \text{(D-1)}$$

The term $\Sigma S_{u,irx}$ or $\Sigma\Delta Q_{irx}k_{irx}$ that appears in the energy balance as a heat source should not be included because it is implicitly included in the terms representing the change of energy of the different components (products and reactants). To show that this term should not be included in the energy equation, consider an isolated closed system with no heat or mass exchange with the surroundings. For such a system, the first law of thermodynamics implies that

$$\Delta U_\sigma=0 \quad \text{(D-2a)}$$

or $$U_{\sigma(\text{final})}-U_{\sigma(\text{initial})}=0, \quad \text{(D-2b)}$$

where U_σ = internal energy of the system. When applied to such a system, the energy balance given by Oballa *et al.* reduces to

$$\Delta U_\sigma=\Sigma S_{u,irx}(\Delta t/V), \quad \text{(D-3)}$$

where U_σ = internal energy of the system including rock and fluids. So

$$U_{\sigma(\text{final})}-U_{\sigma(\text{initial})}\neq 0,$$

which clearly violates the first law of thermodynamics because energy is not conserved.

Eqs. D-2 do not mean, however, that the initial and final states of the system (products and reactants) are at the same temperature. The heat of reaction, ΔQ, is defined as the difference between the enthalpies of reactants and products in proportion to their stoichiometric coefficients,

$$\Delta Q_i=-\sum_{j=1}^{n_c}\alpha_{ij}M_jH_j, \quad \text{(D-4)}$$

where α_{ij} = stoichiometric coefficients of the jth component in the ith reaction (positive for products and negative for reactants), n_c = number of components, M_j = molecular weight of jth component, and H_j = enthalpy of the jth component.

A positive value of ΔQ (exothermic reaction) means that the enthalpy of the generated products is less than the enthalpy of the consumed reactants. This excess of enthalpy results in an increase in the temperature of the components of the system at the final state. This temperature increase causes an increase in the energy of the final state by an amount equal to this excess energy (heat of reaction) so that the total energy of the system is kept constant, as required by the law of conservation of energy.

Clearly, the heat of reaction term $\Sigma S_{u,irx}$ or $\Sigma\Delta Qk$ should not appear in the energy equation presented by the authors.

The inclusion of this term in the energy equation will result in higher values of temperature in the reaction zone. Furthermore, the continuity and energy equations are strongly coupled because most fluid and rock properties as well as the phase-equilibrium constants and reaction rates are temperature-dependent. Inclusion of this term will affect the values of all variables obtained by the numerical solution of the mathematical model.

An alternative form of the energy equation that explicitly includes the heat of reaction term $\Sigma\Delta Q_ik_i$ may be derived by mathematical manipulation of the energy equation and the mass-balance (continuity) equations of the different components of the system. To demonstrate this, the same closed isolated system is considered. For such a system, the continuity equation for the different components is given by

$$\frac{d}{dt}m_j=\sum_{i=1}^{n_{rx}}\alpha_{ij}M_jk_i. \quad \text{(D-5)}$$

If each continuity equation is multiplied by the enthalpy of that component, H_j, and all the resulting equations for the n_c components are added, we get

$$\sum_{j=1}^{n_c}H_j\frac{d}{dt}m_j=\sum_{j=1}^{n_c}H_j\sum_{i=1}^{n_{rx}}\alpha_{ij}M_jk_i$$

$$=\sum_{i=1}^{n_{rx}}k_i\left(\sum_{j=1}^{n_c}\alpha_{ij}M_jH_j\right). \quad \text{(D-6)}$$

We can use the definition of the heat of reaction ΔQ given by Eq. D-4 to write Eq. D-6 as

$$\sum_{j=1}^{n_c}H_j\frac{d}{dt}m_j=-\sum_{i=1}^{n_{rx}}\Delta Q_ik_i. \quad \text{(D-7)}$$

The energy equation for the isolated closed system can be written in the following differential form:

$$\frac{d}{dt}\sum_{j=1}^{n_c}m_jU_j=0. \quad \text{(D-8)}$$

Using chain-rule differentiation and the relation $H=U+pv$, we get

$$\sum_{j=1}^{n_c}m_j\frac{dH_j}{dt}+\sum_{j=1}^{n_c}H_j\frac{dm_j}{dt}=\frac{d}{dt}\left(\sum_{j=1}^{n_c}m_jv_jp\right). \quad \text{(D-9)}$$

Substituting Eq. D-7 into Eq. D-9 gives

$$\sum_{j=1}^{n_c}m_j\frac{dH_j}{dt}=\sum_{i=1}^{n_c}\Delta Q_ik_i+\frac{d}{dt}(pV), \quad \text{(D-10)}$$

where V = total volume of the system, Σm_jv_j.

The last term in Eq. D-10 usually is ignored in most of the energy equations used to simulate thermal processes.

For more complicated models, such as the one used by Oballa *et al.*, the same procedure can be followed. The resulting energy equation, however, will contain terms other than the heat of reaction term, $\Sigma\Delta Q_ik_i$. These additional terms will account for heat of vaporization of the different components of the system. The form and details of derivation of such an equation may be found elsewhere.[5-7]

In conclusion, if the energy equation for systems with chemical reactions is expressed in terms of $(\partial/\partial t)\Sigma(\rho_jS_jU_j)$ and $\nabla\cdot\Sigma(\rho_jv_jH_j)$, it should not include the heat of reaction term $\Sigma\Delta Q_ik_i$. On

the other hand, if the energy equation is expressed in terms of $\Sigma\rho_j S_j(\partial/\partial t)U_j$ and $\nabla\cdot\Sigma\rho_j v_j H_j$, it should include explicitly the term $\Sigma\Delta Q_i k_i$ but with additional terms.

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Authors' Reply to Discussion of Adaptive-Implicit Method in Thermal Simulation

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El-Khatib's discussion on the validity of the energy-balance equation used in our paper appears to be an almost verbatim reproduction of the same discussion point he raised almost a decade ago.[1] Because he has added nothing new to his earlier arguments, we feel the response provided at that time is sufficient.

Reference

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