

Redback Theory Manual

Thomas Poulet
CSIRO

Manolis Vevakis
UNSW

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1. Introduction

The REDBACK application was developed to model multi-physics *Rock mEchanics with Dissipative feedBACKs* in a tightly coupled manner. It is based on the Multi-physics Object Oriented Simulation Environment MOOSE¹ (Gaston et al., 2009) which proposes a powerful and flexible platform to solve multi-physics problems implicitly and in a tightly coupled manner on unstructured meshes. MOOSE aims at providing a wide range of modules to model various physical phenomena, including rock mechanics, which are as flexible as possible and can be easily coupled together. By comparison, REDBACK is The philosophy behind REDBACK is to focus on a non-dimensional formulation of the problem in order to focus on the physical processes at play

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¹<http://mooseframework.org>

2. Governing equations

The system in its final form is

$$\begin{aligned}
 0 &= \partial_j \sigma'_{ij} + \partial_i p_f + b_i, & (2.1a) \\
 0 &= \partial_t p_f + Pe v_i^p \partial_i p_f - Pe v_i^T \partial_i T - \partial_i \left[\frac{1}{Le} \partial_i p_f \right] & (2.1b) \\
 &\quad - \Lambda \partial_t T + \frac{Pe \dot{\epsilon}_V}{\bar{\beta}^*} - \frac{1}{Le_{chem}} \omega_F, \\
 0 &= \partial_t T + Pe \bar{v}_i \partial_i T - \partial_{ii}^2 T - Gr \sigma_{ij}^{pl} \dot{\epsilon}_{ij}^{pl} & (2.1c) \\
 &\quad + Da_{endo} (1-s)(1-\phi) e^{\frac{Ar_F \delta T}{1+\delta T}} \\
 &\quad - Da_{exo} s(1-\phi) \Delta \phi_{chem} e^{\frac{Ar_R \delta T}{1+\delta T}}.
 \end{aligned}$$

All dimensionless groups are defined in Tab. 2.1 and

$$\begin{aligned}
 \bar{\beta} &= (1-\phi)\beta_s + \phi\beta_f, \\
 \bar{\beta}^* &= \bar{\beta} \sigma_{ref}, \\
 v_i^p &= (1-\phi) \frac{\beta_s}{\bar{\beta}} v_i^s + \phi \frac{\beta_f}{\bar{\beta}} v_i^f, \\
 v_i^T &= (1-\phi) \frac{\bar{\lambda}_s}{\bar{\beta}} v_i^s + \phi \frac{\bar{\lambda}_f}{\bar{\beta}} v_i^f, \\
 \bar{v}_i &= \frac{\rho_s}{\bar{\rho}} v_i^s + \frac{\rho_f}{\bar{\rho}} v_i^f, \\
 \omega_F &= (1-\phi)(1-s) \exp \left(\frac{Ar_F \delta T}{1+\delta T} \right), \\
 \omega_R &= (1-\phi) s \Delta \phi_{chem} \exp \left(\frac{Ar_R \delta T}{1+\delta T} \right), \\
 \dot{\epsilon}_{ij}^{pl} &= \dot{\epsilon}_0 \exp \left(\frac{Ar \delta T}{1+\delta T} \right) \sqrt{\left\langle \frac{q - q_Y}{\sigma_{ref}} \right\rangle^{2m} + \left\langle \frac{p - p_Y}{\sigma_{ref}} \right\rangle^{2m}} \frac{\partial f}{\partial \sigma_{ij}}.
 \end{aligned}$$

The total porosity ϕ is expressed as the sum of its initial value, ϕ_0 , and the newly created interconnected pore volume. Pore volume can be created by mechanical ($\Delta \phi_{mech}$) and chemical ($\Delta \phi_{chem}$) processes such that the total porosity reads

$$\phi = \phi_0 + \Delta \phi_{mech} + \Delta \phi_{chem} = \frac{V_B}{V}, \quad (2.2)$$

where V_B is the volume occupied by fluid B . The evolution of mechanical porosity contains two components, a plastic part $\Delta\phi_{mech}^{pl} = \epsilon_V^{pl}$, with ϵ_V^{pl} the volumetric plastic strain, and an elastic one $\Delta\phi_{mech}^e = (1 - \phi)(\beta_s \Delta p_f - \lambda_s \Delta T)$ where β_s and λ_s are compressibility and thermal expansion coefficients of the solid phase, respectively.

2.1. Rescaling

A particularity of REDBACK is to work with dimensionless parameters, in line with the purpose of studying system stabilities. As such, the variables used in the final system of equation (Eq. 2.1) are all dimensionless and defined as such:

$$p^* = \frac{p_f}{\sigma_{ref}}, \quad (2.3a)$$

$$T^* = \frac{T - T_{ref}}{\delta T_{ref}}, \quad (2.3b)$$

$$x^* = \frac{x}{x_{ref}}, \quad (2.3c)$$

$$t^* = \frac{c_{th}}{x_{ref}^2} t, \quad (2.3d)$$

$$V^* = \frac{V}{V_{ref}}. \quad (2.3e)$$

with $c_{th} = \alpha/(\rho C_p)_m$. The derivations of those dimensionless variables is detailed in Sec. A.

Note that the time can in turn be rescaled a second time for numerical reasons (see Sec. 3.1.1).

2.2. Chemical damage

Thermally activated chemical reactions are allowed to take place and in this work we concentrate on (de-)hydration reactions of the form



where the subscripts s and f refer to solid and fluid phases and ν_i ($i = 1, 2, 3$) are stoichiometric coefficients. The reaction equation (2.4) states that the solid A can release/bind the component B into/from the fluid phase which increases/reduces the pore pressure.

The kinetics of the decomposition reaction (2.4) are assumed to follow a standard Arrhenius dependency on temperature (Poulet et al., 2014a). As a result, the rates of the forward, ω_F , and reverse reaction, ω_R (let $\nu_1 = \nu_2 = \nu_3 = 1$) can be expressed as

(Alevizos et al., 2014)

$$\omega_F = \frac{\rho_{AB}}{M_{AB}}(1 - \phi)(1 - s)k_F e^{-Q_F/RT}, \quad (2.5a)$$

$$\omega_R = \frac{\rho_A \rho_B}{M_A M_B}(1 - \phi)s\Delta\phi_{chem}k_R e^{-Q_R/RT}, \quad (2.5b)$$

where ρ_i and M_i ($i = A, B, AB$) are the densities and molar masses of the respective constituent, k_F, k_R, Q_F, Q_R are the pre-exponential factors and activation enthalpies of the forward and reverse reaction, ϕ is porosity and $\Delta\phi_{chem}$ denotes change in porosity due to chemical processes. We define the solid ratio

$$s = \frac{V_A}{V_s} = \frac{V_A}{(1 - \phi)V}, \quad (2.6)$$

where V is a representative volume, V_A and V_s is the volume of solid phase A and all solid within V , respectively. The solid ratio is a measure of the extend of reaction (2.4). Subsequently, the total reaction rate is

$$\omega = \left[(1 - s) - s\Delta\phi_{chem} \frac{\rho_A \rho_B}{\rho_{AB}^2} \frac{M_{AB}^2}{M_A M_B} K_c^{-1} e^{\Delta h/RT} \right] (1 - \phi) \frac{\rho_{AB}}{M_{AB}} k_F e^{-Q_F/RT} \quad (2.7)$$

where $K_c = k_F/k_R$ and $\Delta h = Q_R - Q_F$. The expressions for the dependency of the porosity ϕ and solid ratio s on the reaction kinetics are described in detail in Alevizos et al. (2014) and briefly summarized here.

We assume the following relations for the partial molar reaction rates of the species involved

$$\omega_{AB} = - \left[\frac{\rho_{AB}}{M_{AB}}(1 - \phi)(1 - s) \right]^{\nu_1} k_F \exp(-Q_F/RT), \quad (2.8a)$$

$$\omega_A = \left[\frac{\rho_A}{M_A}(1 - \phi)s \right]^{\nu_2} k_A \exp(-Q_R/RT), \quad (2.8b)$$

$$\omega_B = \left[\Delta\phi_{chem} \frac{\rho_B}{M_B} \right]^{\nu_3} k_B \exp(-Q_R/RT), \quad (2.8c)$$

and those rates are linked by the stoichiometry of the considered reaction (2.4) as

$$- \frac{\omega_{AB}}{\nu_1} = \frac{\omega_A}{\nu_2} = \frac{\omega_B}{\nu_3}. \quad (2.9)$$

From Eqs. (2.8-2.9) and for $\nu_1 = \nu_2 = \nu_3 = 1$ we derive the poro-chemical model

$$\Delta\phi_{chem} = A_\phi \frac{1 - \phi_0}{1 + \frac{\rho_B}{\rho_A} \frac{M_A}{M_B} \frac{1}{s}}, \quad (2.10a)$$

$$s = \frac{\omega_{rel}}{1 + \omega_{rel}}, \quad (2.10b)$$

$$\omega_{rel} = \frac{\rho_{AB}}{\rho_A} \frac{M_A}{M_{AB}} K_c \exp\left(\frac{\Delta h}{RT}\right), \quad (2.10c)$$

where A_ϕ is a coefficient that determines the amount of the interconnected pore-volume (porosity) created due to the reaction. We assume that all the fluid generated contributes to the interconnected pore volume, and thus set $A_\phi = 1$.

Damkohler numbers to check

Table 2.1.: Dimensionless parameters used in REDBACK. The coefficient δ is defined such that $T^* = (T - T_{ref})/(\delta T_{ref})$

Group	Name	Definition	Interpretation
Gr	Gruntfest number	$\frac{\chi \sigma_{ref} \dot{\epsilon}_{ref} x_{ref}^2}{\alpha \delta T_{ref}}$	ratio of mechanical rate converted into over rate of diffusive processes
Da_{endo}	Endothermic Damköhler number	$\frac{A_{endo} h_{endo} \rho_{AB} x_{ref}^2}{\alpha \delta T_{ref}}$	ratio of endothermic reaction rate over rate of diffusive processes
Da_{exo}	Exothermic Damköhler number	$\frac{A_{exo} h_{exo} \rho_{AB} x_{ref}^2}{\alpha \delta T_{ref}}$	ratio of exothermic reaction rate over rate of diffusive processes
Ar	Arrhenius number	$Q_{mech}/(RT_{ref})$	Ratio of activation energy over thermal energy
Ar_F	Forward Arrhenius number	$Q_F/(RT_{ref})$	Ratio of activation energy of forward reaction over thermal energy
Ar_R	Reverse Arrhenius number	$Q_R/(RT_{ref})$	Ratio of activation energy of reverse activation energy over thermal energy
Le	Lewis number	$c_{th}/c_{hy} = \frac{\mu_f c_{th} \beta_m^*}{k \sigma_{ref}}$	Ratio of thermal over mass diffusivities
Le_{chem}	Chemical Lewis number	$\frac{c_{th} \sigma_{ref} \beta_m}{x_{ref}^2 A_{endo}} \frac{\rho_B}{\rho_{AB}} \frac{M_{AB}}{M_B} \left(\frac{\rho_B}{\rho_f} - \frac{\rho_B}{\rho_s} \right) e^{-Ar_F}$	Ratio of thermal over chemical diffusivities for forward reaction
$\bar{\Lambda}$	Thermal pressurisation coefficient	$\frac{\lambda_m}{\beta_m} \frac{\delta T_{ref}}{\sigma_{ref}}$	Normalised thermal pressurisation coefficient with λ_m and β_m the mixture thermal expansion and compressibility
Pe	Péclet number	$x_{ref} V_{ref}/c_{th}$	Ratio of temperature advection rate over diffusion rate

3. Code architecture

3.1. Kernels

Here is the list of all kernels implemented in REDBACK to solve the system of Eq. 2.1:

$$\begin{aligned}
 0 &= \overbrace{\partial_j \sigma'_{ij} + \partial_i p_f + b_i}^{\text{RedbackStressDivergenceTensor}}, \\
 0 &= \underbrace{\partial_t p_f}_{\text{TimeDerivative}} + \underbrace{Pe \bar{v}_i^p \partial_i p_f - Pe \bar{v}_i^T \partial_i T}_{\text{RedbackMassConvection}} - \underbrace{\partial_i \left[\frac{1}{Le} \partial_i p_f \right]}_{\text{RedbackMassDiffusion}} \\
 &\quad - \underbrace{\Lambda \partial_t T}_{\text{RedbackThermalPressurization}} + \underbrace{\frac{Pe \epsilon \dot{V}}{\bar{\beta} \sigma_{ref}}}_{\text{RedbackPoromechanics}} - \underbrace{\frac{1}{Le_{chem}} \omega_F}_{\text{RedbackChemPressure}}, \\
 0 &= \underbrace{\partial_t T}_{\text{TimeDerivative}} + \underbrace{Pe \bar{v}_i \partial_i T}_{\text{RedbackThermalConvection}} - \underbrace{\partial_{ii}^2 T}_{\text{RedbackThermalDiffusion}} - \underbrace{Gr \sigma_{ij}^{pl} \dot{\epsilon}_{ij}^{pl}}_{\text{RedbackMechDissip}} + \underbrace{Da_{endo} \omega_F}_{\text{RedbackChemEndo}} - \underbrace{Da_{exo} \omega_R}_{\text{RedbackChemExo}}.
 \end{aligned}$$

Note that this expression of the system of equation does not include the time rescaling factor (see following Sec. 3.1.1), which explains the presence of a RedbackThermalDiffusion kernel instead of using the default Diffusion kernel from MOOSE.

3.1.1. Time rescaling

The time used in REDBACK is dimensionless and defined in Eq. 2.3. For numerical reasons however, it can sometimes be useful to rescale time again by introducing t' such that

$$t^* = t' \times \text{time_factor}. \quad (3.1)$$

Using the newly defined time t' is equivalent to multiplying all the kernels, other than the time derivatives, of Eq. 2.1b and Eq. 2.1c by *time_factor*. This functionality is required

for cases when the initial residual computation is too low and prevents MOOSE from converging to an accurate solution. It is convenient in those cases (e.g. for convection simulations) to use a large factor *time_factor* to increase the initial value of the residual and therefore allow MOOSE to improve that residual down to a low value which will ensure enough numerical precision.

The *time_factor* is defined for each kernel concerned but should only be input as a global variable in your input file.

```
[GlobalParams]
  time_factor = 1.e-3
[]
```

Note that the real time t is then related to the time t' used in the REDBACK simulations by

$$t = \text{time_factor} \times \frac{x_{ref}^2}{c_{th}} t' \quad (3.2)$$

3.2. Porosity

Porosity plays a particular role as its evolution depends on the mechanical, thermal, and hydraulic process models. As such, the total porosity evolution can not be handled within a material class unfortunately since it has components updated in more than one material. With the RedbackMechMaterial class already derived from the RedbackMaterial class, we can not create a dependency the other way around as it would create a circular dependency problem. There are at least two ways of working around that problem:

1. Porosity can be treated as an extra variable to solve for.
2. Porosity can be treated as an AuxKernel, which allows us to update it with various components calculated in separate material, and yet have all materials use the total porosity (updated with delay obviously).

In the first case the porosity evolution (and dependency on all process models) will be solved rigorously, but this will come at a greater computational cost. This is probably the neatest solution to handle the most generic case when porosity might be strongly dependent on all process models, but this is not the principal scenario we are aiming with the current development of Redback. We are indeed focusing on the case described in Sec. 2, where the porosity is much more strongly dependent on chemistry (which produces fluid and can therefore raise ϕ to 1) than it is on temperature and pore pressure (inducing minor variations of ϕ). As a result, we decided to implement the second option and handle the total porosity as an AuxVariable updated by an AuxKernel. This option provides more flexibility to compute the total porosity more or less accurately by updating the AuxKernel more or less frequently. At the moment we're treating the porosity in an explicit manner and only update it at the end of each step. This is equivalent to say that we neglect the mechanical update of the porosity during a single

step and only consider its chemical variation (since it is the main evolution for the cases we consider).

4. Tests

REDBACK is tested through a series of tests based on various benchmarks for all physical processes involved: thermal (**T**), hydraulic (**H**), mechanical (**M**), and chemical (**C**). All tests are found in the `redback/tests` directory

4.1. Benchmark 1 - T

This benchmark (`redback/tests/benchmark_1_T`) looks at the temperature equation

$$\frac{\partial T}{\partial t} = \frac{\partial^2 T}{\partial x^2} + Gr.e^{\frac{Ar.\delta.T}{1+\delta.T}}. \quad (4.1)$$

The steady state solution is a generalisation of the classical Bratu problem (Bratu, 1914) and is controlled by the Gruntfest number Gr . Using a bifurcation method (Suc-combe, 2015) we can find the critical value of the Gruntfest number as shown on Fig. 4.1

This problem is then solved using MOOSE on a generated 1D mesh from -1 to 1 for different values of Gr and the initial solution of the temperature T_0 in the center:

- $Gr = 0.095$ and $T_0 = 0$. In this case, the system should converge increasingly to a centre temperature $T_a \approx 0.109$. This case is treated with the input file `bench1_a.i`
- $Gr = 0.095$ and $T_0 = 0.15$. In this case, the system should converge decreasingly to the same centre temperature $T_b = T_a \approx 0.109$. This case is treated with the input file `bench1_b.i`
- $Gr = 0.095$ and $T_0 = 0.25$. In this case, the system should converge increasingly to a large temperature $T_c > 1000$. This case is treated with the input file `bench1_c.i`
- $Gr = 0.1$ and $T_0 = 0$. In this case, the system should converge increasingly to an even larger temperature $T_d > T_c > 1000$. This case is treated with the input file `bench1_d.i`

The numerical results match the theory with the time evolutions shown on Fig. 4.2.

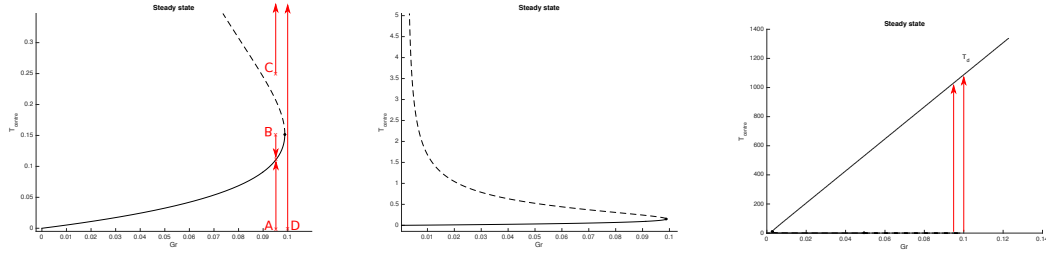


Figure 4.1.: "S-curve" of the steady state analysis for **benchmark_1-T** with a) zoom on low values of temperatures, showing the four starting conditions and their expected time evolution, b) zoomed out view of the unsteady branch of the "S-curve" in dashed line, and c) even more zoomed out view for larger values of temperatures, showing the higher steady branch where benchmarks C and D converge.

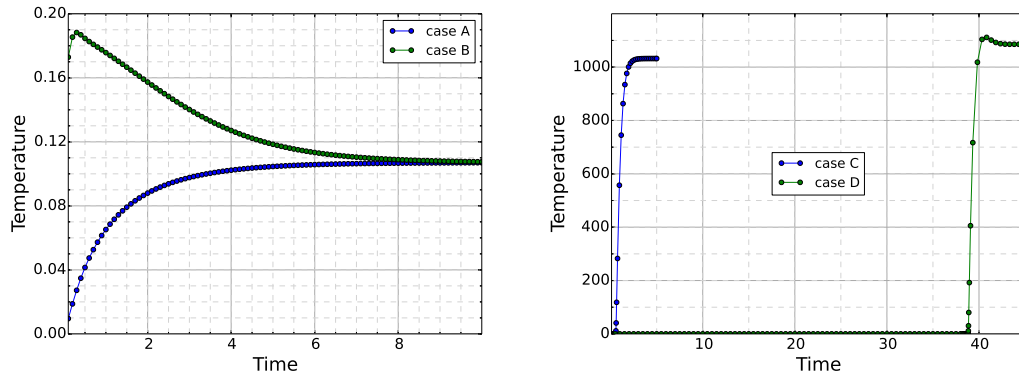


Figure 4.2.: Time evolution of the numerical results for the four benchmarks: a) cases A and B converge to the lower stable branch (see Fig. 4.1), while b) cases C and D converge to the upper stable branch.

A. Derivations

This chapter documents some of the derivations used to obtain the equations presented in Sec.2.

A.1. Mass balance

We define the following densities

$$\rho_1 = (1 - \phi)\rho_s \quad (\text{A.1a})$$

$$\rho_2 = \phi \rho_f \quad (\text{A.1b})$$

and we use the usual material derivative definition

$$\frac{D^{(i)}}{Dt} = \frac{\partial}{\partial t} + v_k^{(i)} \frac{\partial}{\partial x_k} \quad (\text{A.2})$$

Mass balance for the fluid phase

$$\frac{\partial \rho_2}{\partial t} + \frac{\partial(\rho_2 V_k^{(2)})}{\partial x_k} = j_1 \quad (\text{A.3})$$

Using Eq. A.1b in Eq. A.3 we get

$$\phi \frac{\partial \rho_f}{\partial t} + \rho_f \frac{\partial \phi}{\partial t} + \rho_f \frac{\partial(\phi V_k^{(2)})}{\partial x_k} + \phi V_k^{(2)} \frac{\partial \rho_f}{\partial x_k} = j_1 \quad (\text{A.4})$$

Dividing by ρ_f we obtain

$$\frac{\phi}{\rho_f} \frac{D^{(2)} \rho_f}{Dt} + \frac{\partial \phi}{\partial t} + \frac{\partial(\phi V_k^{(2)})}{\partial x_k} = \frac{j_1}{\rho_f} \quad (\text{A.5})$$

Mass balance for the solid phase

$$\frac{\partial \rho_1}{\partial t} + \frac{\partial(\rho_1 V_k^{(1)})}{\partial x_k} = -j_1 \quad (\text{A.6})$$

Using Eq. A.1a in Eq. A.6 we get

$$(1 - \phi) \frac{\partial \rho_s}{\partial t} - \rho_s \frac{\partial \phi}{\partial t} + \rho_s \frac{\partial((1 - \phi) V_k^{(1)})}{\partial x_k} + (1 - \phi) V_k^{(1)} \frac{\partial \rho_s}{\partial x_k} = -j_1 \quad (\text{A.7})$$

Dividing by ρ_s we obtain

$$\frac{(1-\phi)}{\rho_s} \frac{D^{(1)}\rho_s}{Dt} - \frac{\partial\phi}{\partial t} + \frac{\partial(V_k^{(1)})}{\partial x_k} - \frac{\partial(\phi V_k^{(1)})}{\partial x_k} = -\frac{j_1}{\rho_s} \quad (\text{A.8})$$

Mass balance for the mixture (solid + fluid)

Adding Eq. A.5 and Eq. A.8 gives the mixture mass balance:

$$\frac{(1-\phi)}{\rho_s} \frac{D^{(1)}\rho_s}{Dt} + \frac{\phi}{\rho_f} \frac{D^{(2)}\rho_f}{Dt} + \frac{\partial(\phi(V_k^{(2)} - V_k^{(1)}))}{\partial x_k} + \frac{\partial(V_k^{(1)})}{\partial x_k} = \left(\frac{1}{\rho_f} - \frac{1}{\rho_s}\right) j_1 \quad (\text{A.9})$$

Equation of state (EOS)

$$\frac{d\rho_{(i)}}{\rho_{(i)}} = \left(\frac{d\rho_{(i)}}{dp_f}\right)_T \frac{dp_f}{\rho_{(i)}} + \left(\frac{d\rho_{(i)}}{dT}\right)_p \frac{dT}{\rho_{(i)}}, \quad i \in \{s, f\} \quad (\text{A.10})$$

Using the definition for compressibility $\beta_{(i)} = \frac{1}{\rho_{(i)}} \left(\frac{d\rho_{(i)}}{dp_f}\right)_T$ and thermal expansion $\lambda_{(i)} = -\frac{1}{\rho_{(i)}} \left(\frac{d\rho_{(i)}}{dT}\right)_p$ we get the Equation of State (EOS)

$$\frac{d\rho_{(i)}}{\rho_{(i)}} = \beta_{(i)} dp_f - \lambda_{(i)} dT, \quad i \in \{s, f\} \quad (\text{A.11})$$

Using Eq. A.11 in Eq. A.9 leads to

$$(1-\phi) \left[\beta_s \frac{D^{(1)}p_f}{Dt} - \lambda_s \frac{D^{(1)}T}{Dt} \right] + \phi \left[\beta_f \frac{D^{(2)}p_f}{Dt} - \lambda_f \frac{D^{(2)}T}{Dt} \right] + \frac{\partial(\phi(V_k^{(2)} - V_k^{(1)}))}{\partial x_k} + \frac{\partial(V_k^{(1)})}{\partial x_k} = \left(\frac{1}{\rho_f} - \frac{1}{\rho_s}\right) j_1 \quad (\text{A.12})$$

Rearranging the terms we get

$$\begin{aligned} & \overbrace{[(1-\phi)\beta_s + \phi\beta_f]}^{\beta_m} \frac{\partial p_f}{\partial t} - \overbrace{[(1-\phi)\lambda_s + \phi\lambda_f]}^{\lambda_m} \frac{\partial T}{\partial t} \\ & + \left[(1-\phi)\beta_s V_k^{(1)} + \phi\beta_f V_k^{(2)} \right] \frac{\partial p_f}{\partial x_k} - \left[(1-\phi)\lambda_s V_k^{(1)} + \phi\lambda_f V_k^{(2)} \right] \frac{\partial T}{\partial x_k} \\ & + \frac{\partial(\phi(V_k^{(2)} - V_k^{(1)}))}{\partial x_k} + \frac{\partial(V_k^{(1)})}{\partial x_k} = \left(\frac{1}{\rho_f} - \frac{1}{\rho_s}\right) j_1 \quad (\text{A.13}) \end{aligned}$$

Normalisation

In order to deal with dimensionless parameters we introduce the following normalised variables

$$p^* = \frac{p_f}{\sigma_{ref}}, \quad (\text{A.14a})$$

$$T^* = \frac{T - T_{ref}}{\delta T_{ref}}, \quad (\text{A.14b})$$

$$x^* = \frac{x}{x_{ref}}, \quad (\text{A.14c})$$

$$t^* = \frac{c_{th}}{x_{ref}^2} t, \quad (\text{A.14d})$$

$$V^* = \frac{V}{V_{ref}}. \quad (\text{A.14e})$$

Dividing Eq. A.13 by β_m and switching to the normalised variables we get

$$\begin{aligned} & \frac{\sigma_{ref} c_{th}}{x_{ref}^2} \frac{\partial p^*}{\partial t^*} - \frac{\lambda_m \delta T_{ref} c_{th}}{\beta_m x_{ref}^2} \frac{\partial T^*}{\partial t^*} \\ & + \frac{V_{ref} \sigma_{ref}}{x_{ref}} \left[\frac{(1 - \phi) \beta_s V_k^{*(1)} + \phi \beta_f V_k^{*(2)}}{\beta_m} \right] \frac{\partial p^*}{\partial x_k^*} \\ & - \frac{V_{ref} \delta T_{ref}}{x_{ref}} \left[\frac{(1 - \phi) \lambda_s V_k^{*(1)} + \phi \lambda_f V_k^{*(2)}}{\beta_m} \right] \frac{\partial T^*}{\partial x_k^*} \\ & + \frac{V_{ref}}{\beta_m x_{ref}} \frac{\partial(\phi(V_k^{*(2)} - V_k^{*(1)}))}{\partial x_k^*} + \frac{V_{ref}}{\beta_m x_{ref}} \frac{\partial(V_k^{*(1)})}{\partial x_k^*} = \frac{1}{\beta_m} \left(\frac{1}{\rho_f} - \frac{1}{\rho_s} \right) j_1 \quad (\text{A.15}) \end{aligned}$$

This can be rewritten as

$$\begin{aligned} & \frac{\partial p^*}{\partial t^*} - \frac{\overbrace{\lambda_m \delta T_{ref}}^{\Lambda}}{\beta_m \sigma_{ref}} \frac{\partial T^*}{\partial t^*} + \frac{\overbrace{x_{ref} V_{ref}}^{Pe}}{c_{th}} \left[\frac{\overbrace{(1 - \phi)(\sigma_{ref} \beta_s) V_k^{*(1)} + \phi(\sigma_{ref} \beta_f) V_k^{*(2)}}^{\vec{v}^P}}{\sigma_{ref} \beta_m} \right] \frac{\partial p^*}{\partial x_k^*} \\ & - \frac{\overbrace{x_{ref} V_{ref}}^{Pe}}{c_{th}} \left[\frac{\overbrace{(1 - \phi)(\delta T_{ref} \lambda_s) V_k^{*(1)} + \phi(\delta T_{ref} \lambda_f) V_k^{*(2)}}^{\vec{v}^T}}{\sigma_{ref} \beta_m} \right] \frac{\partial T^*}{\partial x_k^*} \\ & + \frac{x_{ref} V_{ref}}{c_{th} \beta_m \sigma_{ref}} \frac{\partial}{\partial x_k^*} \left[\underbrace{\phi(V_k^{*(2)} - V_k^{*(1)})}_{\text{norm. filtration vec.}} \right] + \underbrace{\frac{x_{ref} V_{ref}}{c_{th}}}_{Pe} \underbrace{\frac{1}{\beta_m \sigma_{ref}}}_{\dot{\epsilon}_V^*} \frac{\partial(V_k^{*(1)})}{\partial x_k^*} \\ & = \frac{x_{ref}^2}{\beta_m \sigma_{ref} c_{th}} \left(\frac{1}{\rho_f} - \frac{1}{\rho_s} \right) j_1 \quad (\text{A.16}) \end{aligned}$$

with

$$\Lambda = \frac{\lambda_m \delta T_{ref}}{\beta_m \sigma_{ref}} = \frac{\lambda_m^*}{\beta_m^*}, \quad (\text{A.17a})$$

$$\lambda_i^* = \delta T_{ref} \lambda_i, \quad i \in \{s, f, m\} \quad (\text{A.17b})$$

$$\beta_i^* = \beta \sigma_{ref}, \quad i \in \{s, f, m\} \quad (\text{A.17c})$$

$$Pe = \frac{x_{ref} V_{ref}}{c_{th}}, \quad (\text{A.17d})$$

$$v^p = \frac{(1 - \phi) \beta_s^* V_k^{*(1)} + \phi \beta_f^* V_k^{*(2)}}{\beta_m^*}, \quad (\text{A.17e})$$

$$v^T = \frac{(1 - \phi) \lambda_s^* V_k^{*(1)} + \phi \lambda_f^* V_k^{*(2)}}{\beta_m^*}. \quad (\text{A.17f})$$

The filtration vector $\phi(V_k^{(2)} - V_k^{(1)})$ can be expressed using Darcy's law as

$$\phi(V_k^{(2)} - V_k^{(1)}) = -\frac{k}{\mu_f} \left(\frac{\partial p_f}{\partial x_k} - \rho_f g \vec{e}_z \right) \quad (\text{A.18})$$

In its normalised form it becomes

$$\phi(V_k^{*(2)} - V_k^{*(1)}) = -\frac{k}{\mu_f x_{ref} V_{ref}} \left(\frac{\partial p^*}{\partial x_k^*} - \frac{x_{ref}}{\sigma_{ref}} \rho_f g \vec{e}_z \right) \quad (\text{A.19})$$

The mass balance equation then becomes

$$\begin{aligned} & \frac{\partial p^*}{\partial t^*} - \Lambda \frac{\partial T^*}{\partial t^*} + Pe \vec{v}^p \frac{\partial p^*}{\partial x_k^*} - Pe \vec{v}^T \frac{\partial T^*}{\partial x_k^*} \\ & + \frac{\partial}{\partial x_k^*} \left[\underbrace{\frac{k \sigma_{ref}}{\mu_f c_{th} \beta_m^*}}_{1/Le} \left(\frac{\partial p^*}{\partial x_k^*} - \underbrace{\rho_f \frac{x_{ref}}{\sigma_{ref}} g}_{(\rho_f g)^*} \vec{e}_z \right) \right] + \frac{Pe}{\beta_m^*} \dot{\epsilon}_V^* = \frac{x_{ref}^2}{\beta_m \sigma_{ref} c_{th}} \left(\frac{1}{\rho_f} - \frac{1}{\rho_s} \right) j_1 \end{aligned} \quad (\text{A.20})$$

with the Lewis number defined as $Le = \frac{\mu_f c_{th} \beta_m^*}{k \sigma_{ref}}$ and the normalised gravity term $(\rho_f g)^* = \rho_f \frac{x_{ref}}{\sigma_{ref}} g$.

Following (Alevizos et al., 2014, appendix A) $j_1 = \omega_F M_B$, $\omega_F = \frac{\rho_1}{M_{AB}} k_F \exp(-Q_F/RT)$ and $\rho_1 = (1 - \phi)(1 - s)\rho_{AB}$, so the volumetric source term j_1 can be written as

$$j_1 = \rho_{AB} \frac{M_B}{M_{AB}} (1 - \phi)(1 - s) k_F \exp(-Q_F/RT) \quad (\text{A.21})$$

The RHS term of Eq. A.20 can then be written as

$$\begin{aligned} \frac{x_{ref}^2}{\beta_m \sigma_{ref} c_{th}} \left(\frac{1}{\rho_f} - \frac{1}{\rho_s} \right) j_1 &= \frac{x_{ref}^2}{\beta_m \sigma_{ref} c_{th}} \left(\frac{1}{\rho_f} - \frac{1}{\rho_s} \right) \rho_{AB} \frac{M_B}{M_{AB}} (1-\phi)(1-s) k_F \exp(-Q_F/RT) \\ &= \underbrace{\frac{x_{ref}^2 k_F}{\beta_m \sigma_{ref} c_{th}} \frac{\rho_{AB}}{\rho_B} \frac{M_B}{M_{AB}} \left(\frac{\rho_B}{\rho_f} - \frac{\rho_B}{\rho_s} \right)}_{1/L_{chem}} \underbrace{e^{-Ar_F} (1-\phi)(1-s) \exp\left(\frac{Ar_F \delta T^*}{1 + \delta T^*}\right)}_{\omega_F^*} \end{aligned} \quad (\text{A.22})$$

We then arrive to the full mass balance equation Eq. 2.1b

A.2. Energy balance

The local form of the energy balance equation reads as follows:

$$(\rho C_p)_m \frac{D^{(m)}T}{Dt} = \kappa \nabla^2 T + \chi \sigma_{ij} \cdot \dot{\epsilon}_{ij}^p - \Delta H (\omega_F - \omega_R) \quad (\text{A.23})$$

with χ the Taylor-Quinney coefficient and $\Delta H = \Delta E = E_F - E_R$ the reaction's specific enthalpy. The definitions of the reaction rates ω_F and ω_R are (from Eq. 2.7)

$$\omega_F = k_F (1-s)(1-\phi) \frac{\rho_{AB}}{M_{AB}} e^{-Q_F/RT} \quad (\text{A.24a})$$

$$\omega_R = k_R s(1-\phi) \Delta \phi_{chem} \frac{\rho_A \rho_B}{\rho_{AB}} \frac{M_{AB}}{M_A M_B} e^{-Q_R/RT} \quad (\text{A.24b})$$

Using the normalised variable we get

$$\begin{aligned} \frac{\delta T_{ref} c_{th}}{x_{ref}^2} (\rho C_p)_m \frac{\partial T^*}{\partial t^*} &+ \frac{\delta T_{ref} v_{ref}}{x_{ref}} (\rho C_p)_m \bar{v} \cdot \frac{\partial T^*}{\partial x^*} \\ &- \frac{\kappa \delta T_{ref}}{x_{ref}^2} \nabla^2 T - \frac{\sigma_{ref} c_{th}}{x_{ref}^2} \chi \sigma_{ij}^* \cdot \dot{\epsilon}_{ij}^{*(p)} \\ &- \Delta H \cdot k_F (1-s)(1-\phi) \frac{\rho_{AB}}{M_{AB}} e^{-Q_F/RT} \\ &+ \Delta H \cdot k_R s(1-\phi) \Delta \phi_{chem} \frac{\rho_A \rho_B}{\rho_{AB}} \frac{M_{AB}}{M_A M_B} e^{-Q_R/RT} = 0 \end{aligned} \quad (\text{A.25})$$

Note that the reference strain rate is also rescaled so

$$\dot{\epsilon}_0^* = \dot{\epsilon}_0 \frac{x_{ref}^2}{c_{th}} \quad (\text{A.26})$$

This leads to

$$\begin{aligned}
\frac{\partial T^*}{\partial t^*} + \underbrace{\frac{Pe}{x_{ref} v_{ref}}}_{c_{th}} \bar{v} \cdot \frac{\partial T^*}{\partial x^*} - \underbrace{\frac{\kappa}{(\rho C_p)_m}}_{c_{th}} \frac{1}{c_{th}} \nabla^2 T - \underbrace{\frac{\sigma_{ref}}{\delta T_{ref} (\rho C_p)_m}}_{Gr} \chi \sigma_{ij}^* \cdot \dot{\epsilon}_{ij}^{*(p)} \\
- \underbrace{\frac{\Delta H x_{ref}^2 k_F}{\delta T_{ref} \kappa} \frac{\rho_{AB}}{M_{AB}} e^{-Ar_F} (1-s)(1-\phi) e^{\frac{Ar_F \delta T^*}{1+\delta T^*}}}_{Da_{endo}} \\
+ \underbrace{\frac{\Delta H x_{ref}^2 k_R}{\delta T_{ref} \kappa} \frac{\rho_{AB}}{\rho_{AB}} \frac{M_{AB}}{M_A M_B} e^{-Ar_R} s(1-\phi) \Delta \phi_{chem} e^{\frac{Ar_R \delta T^*}{1+\delta T^*}}}_{Da_{exo}} = 0 \quad (A.27)
\end{aligned}$$

and finally to Eq. 2.1c

A.3. Jacobians

Numerical convergence can be helped by providing the jacobians and off-diagonal terms for the kernel residuals, even though MOOSE does not explicitly require them. It is a trial-and-error process to check if the improvement in convergence justifies the cost of computing those terms. See the MOOSE workshop manual on <http://mooseframework.org/documentation/> for more details.

If $R(u)$ is the residual for the variable u , the jacobian matrix J is defined as

$$J_{ij}(u) = \frac{\partial R_i(u)}{\partial u_j} \quad (A.28)$$

and the off-diagonal jacobian term for another coupled variable v as

$$J_{ij}^{(\text{off diag})}(u) = \frac{\partial R_i(u)}{\partial v_j} \quad (A.29)$$

A.3.1. RedbackMassConvection

The residual is defined as

$$R = Pe v^p \cdot \nabla p^* - Pe v^T \cdot \nabla T^* \quad (A.30)$$

with (see Eq.2.1)

$$\begin{aligned}
v_i^p &= (1-\phi) \frac{\beta_s^*}{\beta_m^*} v_i^{*(s)} + \phi \frac{\beta_f^*}{\beta_m^*} v_i^{*(f)}, \\
v_i^T &= (1-\phi) \frac{\lambda_s^*}{\beta_m^*} v_i^{*(s)} + \phi \frac{\lambda_f^*}{\beta_m^*} v_i^{*(f)}.
\end{aligned}$$

Noting that $\frac{\partial \nabla u}{\partial u_j} = \nabla \phi_j$ for any variable u (see MOOSE documentation),

$$J = \frac{\partial R}{\partial p^*} = Pe \frac{\partial v^p}{\partial p^*} \cdot \nabla p^* + Pe v^p \nabla \phi_j - Pe \frac{\partial v^T}{\partial p^*} \cdot \nabla T^* \quad (\text{A.31})$$

The normalised filtration vector (Eq. A.19) can be rewritten as

$$\phi(v^{*(f)} - v^{*(s)}) = -\frac{\beta_m^*}{Le Pe} (\nabla p^* - \rho_f g^*) \quad (\text{A.32})$$

Deriving that equation and adding the equation of state (Eq. A.11) we get

$$\frac{\partial(\phi v^{*(f)})}{\partial p^*} = -\frac{\beta_m^*}{Le Pe} (\nabla \phi_j - \beta_f^* \rho_f g^*) \quad (\text{A.33})$$

under the following simplifying assumptions:

- $\frac{\partial v^{(s)}}{\partial p^*} = 0$
- $\frac{\partial \mu_f}{\partial p^*} = 0$
- $\frac{\partial \phi}{\partial p^*} = 0$

Using $\frac{\partial \rho_f}{\partial p^*} = \beta_f^* \rho_f$ we get

$$\frac{\partial v^p}{\partial p^*} = -\frac{\beta_f^*}{Le Pe} (\nabla \phi_j - \beta_f^* \rho_f g^*) \quad (\text{A.34a})$$

$$\frac{\partial v^T}{\partial p^*} = -\frac{\lambda_f^*}{Le Pe} (\nabla \phi_j - \beta_f^* \rho_f g^*) \quad (\text{A.34b})$$

Eq. A.31 then becomes

$$\begin{aligned} J &= Pe \frac{\partial v^p}{\partial p^*} \cdot \nabla p^* + Pe v^p \nabla \phi_j - Pe \frac{\partial v^T}{\partial p^*} \cdot \nabla T^* \\ &= -\frac{1}{Le} (\nabla \phi_j - \beta_f^* \rho_f g^*) (\beta_f^* \nabla p^* - \lambda_f^* \nabla T^*) + Pe v^p \nabla \phi_j \\ &= \left(Pe v^p - \frac{1}{Le} (\beta_f^* \nabla p^* - \lambda_f^* \nabla T^*) \right) \nabla \phi_j + \frac{1}{Le} \beta_f^* \rho_f g^* (\beta_f^* \nabla p^* - \lambda_f^* \nabla T^*) \end{aligned} \quad (\text{A.35a})$$

Using $\frac{\partial \rho_f}{\partial T^*} = -\lambda_f^* \rho_f$ we get

$$\frac{\partial v^p}{\partial T^*} = -\frac{\beta_f^* \lambda_f^*}{Le Pe} \rho_f g^* \quad (\text{A.36a})$$

$$\frac{\partial v^T}{\partial T^*} = -\frac{\lambda_f^{*2}}{Le Pe} \rho_f g^* \quad (\text{A.36b})$$

$$(\text{A.36c})$$

The off-diagonal jacobian with respect to temperature is defined as

$$\begin{aligned} J^T &= \frac{\partial R}{\partial T^*} = Pe \frac{\partial v^p}{\partial T^*} \cdot \nabla p^* - Pe \frac{\partial v^T}{\partial T^*} \nabla T^* - Pe v^T \cdot \nabla \phi_j \\ &= -\frac{\lambda_f^*}{Le} \rho_f g^* (\beta_f^* \nabla p^* - \lambda_f^* \nabla T^*) - Pe v^T \cdot \nabla \phi_j \end{aligned} \quad (\text{A.37a})$$

A.3.2. RedbackThermalConvection

The residual is defined as

$$R = Pe \bar{v} \cdot \nabla T^* \quad (\text{A.38})$$

and the corresponding jacobian as

$$J = \frac{\partial R}{\partial T^*} = Pe \frac{\partial \bar{v}}{\partial T^*} \cdot \nabla T^* + Pe \bar{v} \cdot \nabla \phi_j. \quad (\text{A.39})$$

From the definition of the normalised filtration velocity (Eq. A.32) we get

$$\frac{\partial v^{*(f)}}{\partial T^*} = -\frac{\beta_m^* \lambda_f^*}{Le Pe \phi} \rho_f g^* \quad (\text{A.40})$$

From the definition of the mixture barycentric velocity $\bar{v} = \frac{\rho_s}{\bar{\rho}} v^{*(s)} + \frac{\rho_f}{\bar{\rho}} v^{*(f)}$ and following the same assumptions that led to Eq. A.34 we write

$$\begin{aligned} \frac{\partial \bar{v}}{\partial T^*} &= -\frac{1}{\bar{\rho}^2} \frac{\partial \bar{\rho}}{\partial T^*} (\rho_s v^{*(s)} + \rho_f v^{*(f)}) + \frac{1}{\bar{\rho}} \left[\frac{\partial \rho_s}{\partial T^*} v^{*(s)} + \frac{\partial \rho_f}{\partial T^*} v^{*(f)} + \rho_f \frac{\partial v^{*(f)}}{\partial T^*} \right] \quad (\text{A.41a}) \\ &= -\frac{1}{\bar{\rho}} \frac{\partial \bar{\rho}}{\partial T^*} \bar{v} + \frac{1}{\bar{\rho}} \left[\frac{\partial \rho_s}{\partial T^*} v^{*(s)} + \frac{\partial \rho_f}{\partial T^*} v^{*(f)} + \rho_f \frac{\partial v^{*(f)}}{\partial T^*} \right] \\ &= \frac{1}{\bar{\rho}} \left[(1 - \phi) \lambda^{*(s)} \rho_s + \phi \lambda^{*(f)} \rho_s \right] \bar{v} - \frac{1}{\bar{\rho}} \left[\lambda^{*(s)} \rho_s v^{*(s)} + \lambda^{*(f)} \rho_f v^{*(f)} \right] - \frac{\rho_f}{\bar{\rho}} \frac{\beta_m^* \lambda_f^*}{Le Pe \phi} \rho_f g^* \\ &= \dots \\ &= \frac{1}{\bar{\rho}} \left[\lambda_m^* \rho_s \bar{v} - \lambda_s^* \rho_s v^{*(s)} - \lambda_f^* \rho_f v^{*(f)} \right] - \frac{\rho_f}{\bar{\rho}} \frac{\beta_m^* \lambda_f^*}{Le Pe \phi} \rho_f g^* \end{aligned}$$

For the off-diagonal term with respect to pore pressure we get

$$\begin{aligned}
\frac{\partial \bar{v}}{\partial p^*} &= -\frac{1}{\bar{\rho}^2} \frac{\partial \bar{\rho}}{\partial p^*} (\rho_s v^{*(s)} + \rho_f v^{*(f)}) + \frac{1}{\bar{\rho}} \left[\frac{\partial \rho_s}{\partial p^*} v^{*(s)} + \frac{\partial \rho_f}{\partial p^*} v^{*(f)} + \rho_f \frac{\partial v^{*(f)}}{\partial p^*} \right] \quad (\text{A.42a}) \\
&= -\frac{1}{\bar{\rho}} \frac{\partial \bar{\rho}}{\partial p^*} \bar{v} + \frac{1}{\bar{\rho}} \left[\frac{\partial \rho_s}{\partial p^*} v^{*(s)} + \frac{\partial \rho_f}{\partial p^*} v^{*(f)} + \rho_f \frac{\partial v^{*(f)}}{\partial p^*} \right] \\
&= -\frac{1}{\bar{\rho}} \left[(1 - \phi) \beta^{*(s)} \rho_s + \phi \beta^{*(f)} \rho_s \right] \bar{v} + \frac{1}{\bar{\rho}} \left[\beta^{*(s)} \rho_s v^{*(s)} + \beta^{*(f)} \rho_f v^{*(f)} \right] \\
&\quad - \frac{\rho_f}{\bar{\rho}} \frac{\beta_m^*}{Le Pe \phi} (\nabla \phi_j - \beta_f^* \rho_f g^*) \\
&= \dots \\
&= \frac{1}{\bar{\rho}} \left[-\beta_m^* \rho_s \bar{v} + \beta_s^* \rho_s v^{*(s)} + \beta_f^* \rho_f v^{*(f)} \right] - \frac{\rho_f}{\bar{\rho}} \frac{\beta_m^*}{Le Pe \phi} (\nabla \phi_j - \beta_f^* \rho_f g^*)
\end{aligned}$$

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