

Motivation I: Consistency

Approximations in moist thermodynamics of atmospheric/weather models are often inconsistent. Different parts of models may handle the thermodynamics in different ways, or general inconsistencies with the laws of thermodynamics may exist, e.g.

- p^{sat} of water is taken from empirical formula created by fitting data instead of derived from the EoS (Equation of State).
- Specific heat capacity changes due to phase composition.
- Latent heat of vapor L^v is not constant since $C_p^v \neq C^l$.

Motivation II: Flexibility

Changing the equation of state in a model usually proves to be difficult due to hard-coding into many model components.

A switchable EoS could be useful for

- Increasing accuracy of EoS necessary for modelling tropical tropopause region.
- Testing effect of current approximations.
- Exoplanetary conditions, e.g. in gas giants; regions of variable atmospheric composition, such as the thermosphere.

Thermodynamic Potential Solution

To address these problems we begin with a family of thermodynamic potentials, all derived from the EoS. From this all relevant quantities can then be found. This would enforce **consistency**, and increase **flexibility** of the model.

Thermodynamic potentials commonly considered are;

Internal energy	$e(\alpha, \eta, q) = e,$	(1)
Enthalpy	$h(p, \eta, q) = e + \alpha p,$	(2)
Helmholtz	$f(\alpha, T, q) = e - \eta T,$	(3)
Gibbs	$g(p, T, q) = e + \alpha p - \eta T,$	(4)

α : specific volume, η : specific entropy, q : water mass fraction, p : pressure, T : temperature.

The Gibbs is a sensible choice for two-phase systems such as in Thuburn 2017 [3], since in equilibrium for phases a, b ,

$$p_a = p_b \quad T_a = T_b \quad g_a = g_b. \quad (5)$$

When extending this to three phases however **an issue arises!** An ambiguity exists at the triple-point using the Gibbs. Instead, a better choice is **internal energy**.

Modelling Fluxes

Imagine a lagrangian parcel of moist air — potentially containing vapor, liquid, and ice. Components may interact with each another, exchanging mass, volume, energy; and may also interact with the surroundings, exchanging volume and energy. A flux diagram may then be drawn like so,

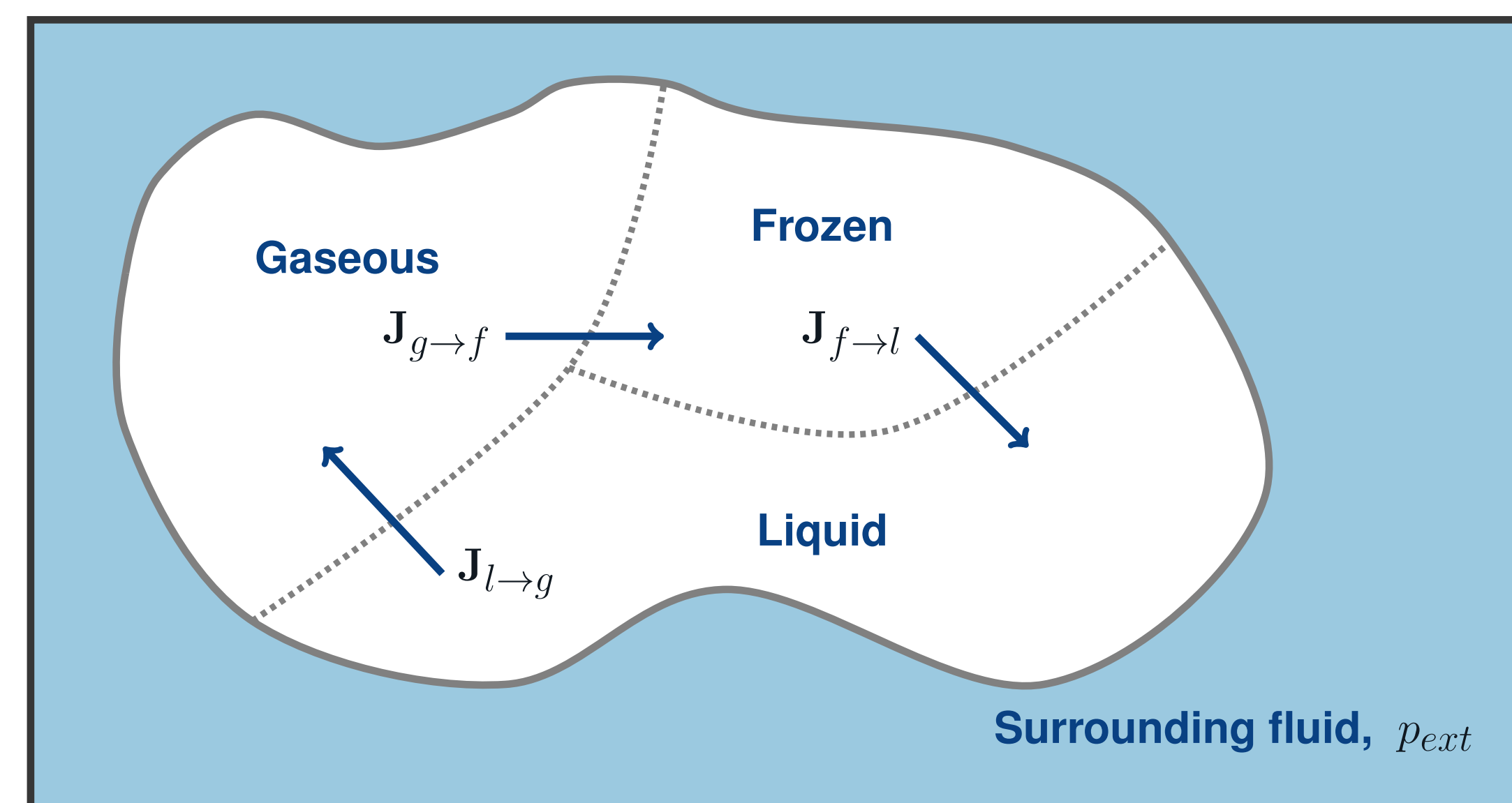


Fig. 1: Lagrangian Parcel Flux Schematic

where each J arrow represents a flux from component a to b which includes the following forms:

$$\text{Mass: } \mathcal{K}_{a \rightarrow b} \quad \text{Energy: } \mathcal{E}_{a \rightarrow b} \quad \text{Volume: } \mathcal{A}_{a \rightarrow b}.$$

Using Onsager Reciprocal Relations

It turns out that modelling a system in terms of fluxes is very useful. Onsager [2] proposed that the entropy production in all systems obey

$$d\eta = \sum_i J_i X_i \geq 0 \quad (6)$$

where J_i represents the fluxes, and X_i the conjugate forces. The fluxes are linear combinations of *all* forces, i.e.

$$J_i = \sum_j L_{ij} X_j \quad (7)$$

where L_{ij} is a positive semi-definite symmetric matrix of coefficients.

Each flux then may be written as some matrix of coefficients multiplied by the thermodynamic forces of the system, e.g.

$$\begin{pmatrix} \mathcal{E}' \\ \mathcal{K} \end{pmatrix}_{l \rightarrow f} = \mathbf{L}_{l \rightarrow f} \begin{pmatrix} \Delta \left(\frac{1}{T} \right) \\ \Delta \left(\frac{-q}{T} \right) \end{pmatrix}_{l \rightarrow f} \quad (8)$$

determines fluxes from liquid to frozen component.

System of ODEs

After writing out the system fluxes it is possible to express differential equations evolving the various system variables.

In general for the lagrangian parcel

$$\frac{D}{Dt} \mathbf{x} = \mathbf{J} \quad (9)$$

where \mathbf{x} contains the system variables, and \mathbf{J} the collection of fluxes.

By using this and appropriately choosing the \mathbf{L} matrix coefficients (from previous) the system can be solved numerically using a **constrained backward-Euler scheme**.

Rigid Parcel Boundary Model

First, it is interesting to simulate a parcel with rigid walls with no external interactions. Setting the initial conditions to be close to the triple point we can iterate through time and find the bulk evolution of the parcel.

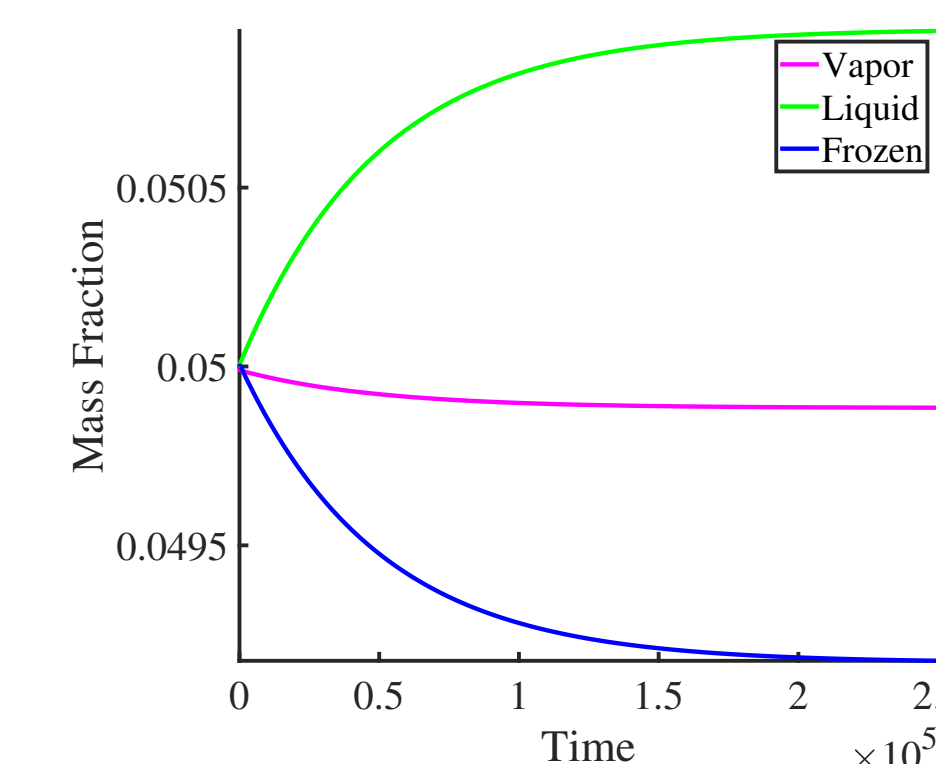


Fig. 2: Non-Equilibrium mode, $\Delta t = 10$

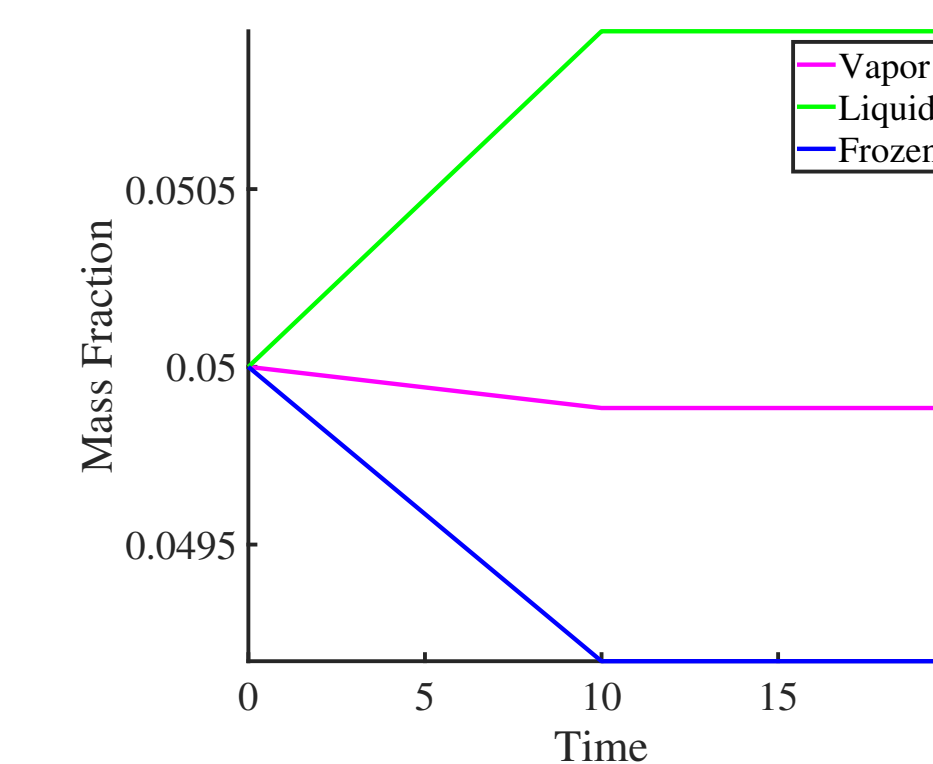


Fig. 3: Equilibrium mode, $\Delta t = 10$

Non-Equilibrium Mode: From initial conditions the system evolves over time to approach a final steady state where all flux transfers become zero.

Equilibrium Mode: Solution is attained on the first time-step, as expected.

Simple Parcel Model

Second, this can be coupled with some rudimentary dynamics in anticipation for coupling to a more complex solver. Write

$$\frac{D\alpha}{Dt} = \dot{\alpha} \quad (10)$$

$$\frac{D\dot{\alpha}}{Dt} = C(p - p_{ext}) \quad (11)$$

where C is some expansion parameter, p_{ext} the external pressure. We can verify the thermodynamic coupling to simple physics under some interesting initial conditions.

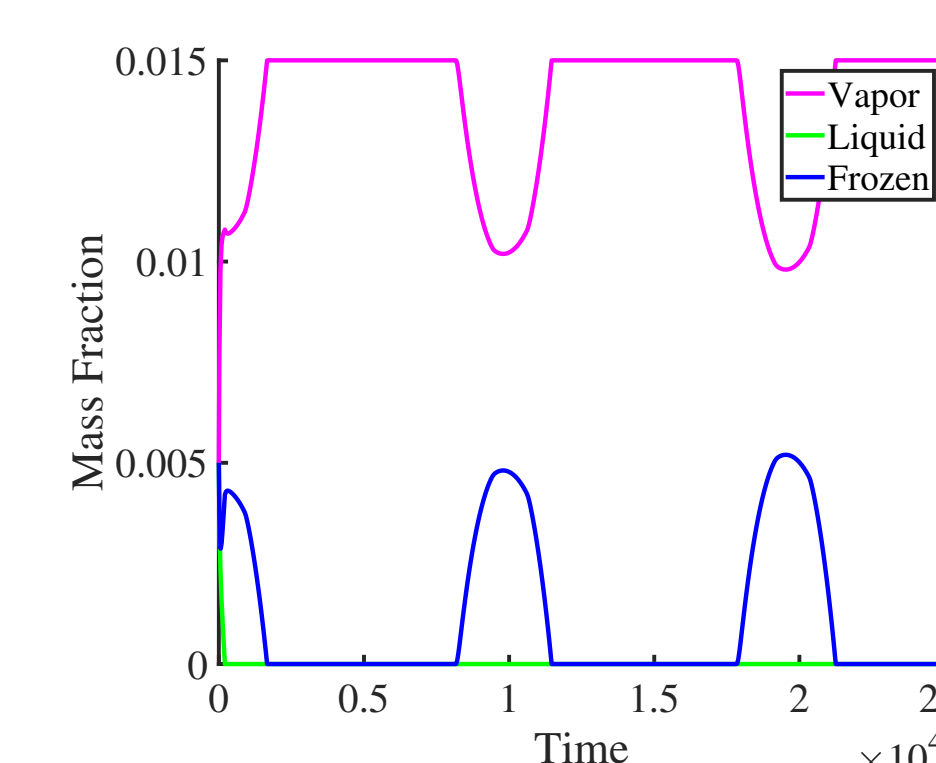


Fig. 4: Phase Fractions

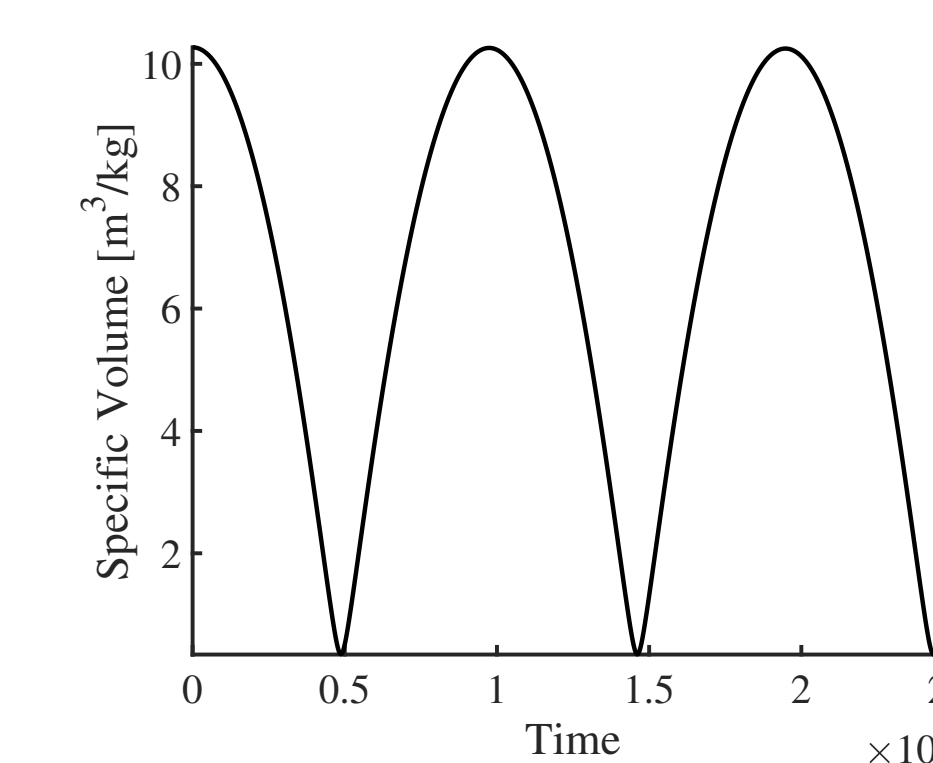


Fig. 5: Parcel Volume

In this case, the lagrangian parcel is observed to elastically expand and contract. As it does so the internal parcel thermodynamics change. By then following the flux principles laid out previously this feeds the internal phase changes. As this is a perfectly elastic model we see this happen cyclically.

Limitations

- Determining the \mathbf{L} coefficients is not entirely straightforward since the relationship between chemical potential difference and phase change rate is not often quantified.
- This so far assumes the entire parcel is a well mixed homogeneous fluid, which is not generally the case in the atmosphere.
- The model presented is inherently more complex than the two-phase case as in Thuburn 2017 [3], solving a larger system at each time-step. As such it is more computationally expensive.

Next Steps

- The \mathbf{L} matrix coefficients must be fully determined from the microphysics.
- To couple a similar system to a 2d dynamical core — this is intended to be a fork of ENDGame.
- Verify simulations against bubble test case of Bryan and Fritsch [1].

Acknowledgements

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References

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