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VENTILATION OF POLLUTANTS TRAPPED IN VALLEYS: A SIMPLE PARAMETERIZATION FOR REGIONAL-SCALE DISPERSION MODELS

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Abstract—Pollutants emitted within a deep valley during night-time can be trapped within the stably stratified valley atmosphere and carried down the valley in locally developed drainage wind systems. After sunrise, as the valley atmosphere becomes heated and destabilized, the night-time pollutant plume is released into the regional-scale flows above the valley. Existing regional-scale transport and diffusion models unable to resolve the local circulations simply approximate pollutant transport during both day and night as a continuous release of pollutants from the source into the regional-scale flows. Regional flows, also, frequently differ in direction from the actual locally developed flows. This, in conjunction with treating the pollutant release to the regional flows as continuous, could result in poor performance of the regional-scale model.

A method is described for parameterizing night-time valley-scale pollutant transport and post-sunrise break-up of the valley plume in regional-scale transport and diffusion models. A conceptual model of the technique is presented and simplified mathematical equations are given to illustrate the technique. Model simulations are presented to show the significant effect of the parameterization on regional-scale ground-level concentrations.

Key word index: Regional-scale dispersion modeling, valley pollution ventilation, complex terrain dispersion modeling, scale interaction, valley temperature inversion break-up.

1. INTRODUCTION

It is well known that local wind circulations regularly form within areas of complex terrain. At night-time, for example, downslope and down-valley flows are caused by cooling and subsequent drainage of cold air into low-lying areas. Deep temperature inversions can form in valleys during the night as cold air builds up over the valley floor. The valley flows become 'decoupled' from the regional flows. Pollutants released in valleys may become trapped within these temperature inversions and carried down-valley in the locally developed mountain–valley circulations (Hewson and Gill, 1944; Sivertsen *et al.*, 1983). During the temperature inversion break-up period after sunrise, air pollutants trapped within the stably stratified air in valleys at night are carried from the valleys and are dispersed in the prevailing regional-scale flows above the valleys. The valley flows during this time period become 'coupled' to the regional flows.

Existing regional-scale models are generally unable to resolve valley circulations explicitly, and therefore simply release pollution from sources located in valleys continuously into the regional-scale flows. This is contrary to the observed behavior of pollution from sources located in valleys, as discussed previously. Therefore, from the point of view of regional-scale dispersion models, deep valleys with pollution sources should be considered as line sources of pollution, where the release rate of pollution to the regional-scale flows is dictated, in some part, by the dynamics of the valley atmosphere.

Some of the implications and unknowns in the above description of coupling and decoupling processes must be stressed. First, these processes do not necessarily occur every day. In fact, they are dependent on the synoptic environment. Strong synoptic winds may modulate or dominate the local circulations. Bell and Thompson (1980), for example, have observed that strong crosswinds may sweep a valley of an initial thermal stratification, thus ventilating the valley. Various synoptic conditions could affect the timing or efficiency of the coupling and decoupling processes. Cloudiness, soil moisture, snow cover, and other factors affecting the surface energy budget also have an important effect on the development and/or destruction of local wind systems and temperature inversions. Also, in terms of regional-scale modeling, coupling and decoupling are concerned with the disposition of pollution emitted in valleys. In some circumstances a continuous elevated plume may be partly carried within local circulations and partly transported by the regional-scale flows.

Despite these complications, we recently developed a simple parameterization of valley coupling and decoupling processes and included it in a regional-scale puff-trajectory model. The interested reader should refer to the detailed technical description and computer code for the MELSAR (Mesoscale Location Specific Air Resources) model (Allwine and Whiteman, 1985) for full information. Following is a description of the salient features of the parameterization, which could be implemented in a trajectory or grid-based regional-scale model. Sample simulations with the MELSAR model are presented to illustrate the method.

2. DESCRIPTION OF THE PARAMETERIZATION

Only valleys that contain pollutant sources in the regional domain are treated. Each such valley is approximated by a series of linear valley segments in which topographic characteristics and inversion characteristics are uniform.

Observations in valleys show that the valley atmosphere typically becomes decoupled from the regional-scale flows above the mountains during a short transition period in the late afternoon or early evening. Daily upper-air data (e.g. U.S. National Weather Service rawinsonde data) from the station nearest the valley are processed to estimate if and when the valley flows become decoupled from the prevailing synoptic flows. During the decoupled period, pollution emitted within the valley is assumed to be carried down the valley in locally developed drainage flows at speeds typical of the valley to be modeled. Thus, at the end of the decoupled period (usually sunrise), the plume is distributed along a length of the valley, down-valley from the pollution source. The plume length is dependent on the duration of the decoupled period and the drainage wind speed. If a valley system has a topographic constriction that blocks down-valley flow, then the plume length would not extend beyond the constriction.

After sunrise, temperature inversion break-up processes cause the plume to be released from the valley into the regional-scale flows throughout the temperature inversion break-up period. The length of this period depends on the thermal energy budget of the valley atmosphere, which, in turn, depends on the strength and depth of the inversion at sunrise and the flux of sensible heat into the valley atmosphere. The surface sensible heat flux depends on Sun–Earth geometry and the characteristics of the surface (e.g. whether snow- or vegetation-covered) and is thus a function of season and, on a given day, soil moisture, presence of snow cover, cloudiness, and other factors. The pollutant release rates from the valley are calculated using simplified pollutant and atmospheric mass budgets for the valley and a temperature inversion break-up model developed by Whiteman and McKee (1982).

In the MELSAR model (Allwine and Whiteman, 1985), the pollution transfer from the valley to the regional scale is accomplished in a puff modeling framework in which pollution is released from valley segments at discrete time intervals. Pollution release rates are computed for each valley segment. In a grid-based model, on the other hand, the pollution from each valley segment can be released directly into the base of the appropriate grid cell.

Computer algorithms that use the rawinsonde data nearest the valley to estimate the effect of day-to-day synoptic conditions on the valley energy budget are incorporated in MELSAR. These algorithms provide a means of determining when the valley coupling and decoupling periods do not follow a normal cycle. For further discussion in this article, we will illustrate the parameterization for the normal situation in which the valley atmosphere becomes decoupled at sunset and becomes recoupled over a period that starts at sunrise.

3. POLLUTION IN THE VALLEY AT SUNRISE

The total amount of pollution in each valley segment at sunrise, M_i, can be estimated by considering that the plume is carried down the valley during the decoupled period τ_D at some mean down-valley wind speed U. The decoupled period for the typical situation is considered to be from sunset on the previous day to sunrise on the current day. The total length of valley, L_T, containing pollution at sunrise would be

$$L_T = U\tau_D. \tag{1}$$

The total valley length may be reduced from this value if a topographic constriction is effective in blocking the drainage flow. Given the pollutant source strength Q_s, the total mass of pollutant in each valley segment of length L_i can be calculated as

$$M_i = Q_s \tau_D \frac{L_i}{L_T}. \tag{2}$$

The lengths of the valley segments must sum to L_T.

Pollution released in the valley at night is assumed to be mixed uniformly through a valley cross-section below the inversion top. This initial assumption is used here to simplify the mathematics. A more general approach has been developed to treat other more realistic vertical (and horizontal) concentration profiles (Whiteman and Allwine, 1985). The assumed nocturnal concentration profiles in the valley can have a significant effect on the post-sunrise regional-scale ground level concentrations, especially regarding the timing of pollutant release from the valley and the concentrations experienced in the immediate vicinity of the valley. This is discussed further in section 5.

At this point, the valley length has been approximated by a series of line segments, and the pollutant mass within each segment is determined at sunrise from Equation (2). The next step in the process is to ascertain how the pollution within the valley segment is released to the regional flow during the temperature inversion break-up period.

4. POLLUTION RELEASED DURING THE INVERSION BREAK-UP PERIOD

Following previous work (Whiteman and McKee, 1982), a valley temperature inversion is considered, in the thermodynamic sense, as representing a thermal energy deficit in the valley relative to the air above the valley. The temperature inversion can be destroyed, and the valley flow coupled to the air above, if enough energy is put into the valley (below the inversion top) to overcome this energy deficit. The energy source used to overcome this deficit is the flux of sensible heat from the valley surfaces after sunrise. This flux can be parameterized as a time-invariant fraction of the extraterrestrial solar heat flux, which varies approximately sinusoidally through the day with a maximum value at solar noon and zero values at sunrise and sunset. Using this concept, Whiteman and McKee (1982) developed a coupled set of equations that predict the depth of the valley temperature inversion, h, and the depth of the convective boundary layer (CBL), H, which forms over the valley floor and sidewalls after sunrise. The prediction equations are given in the Appendix.

These coupled equations are integrated numerically from initial conditions of inversion height, h_0, and CBL height, H_0, at sunrise, using values for the parameters discussed in the Appendix. The integration proceeds for discrete time steps and is completed when the inversion is destroyed. Destruction occurs at the first time step, n, at which the CBL height becomes greater than the inversion top height such that $H_n > h_n$.

Post-sunrise destruction of the nocturnal inversion is accomplished by the upward growth of a CBL into the base of the inversion and the sinking of the inversion top. Upslope flows that develop over the sidewalls are the mechanisms by which stable air entrained into the growing CBLs is removed from the valley. The reduction in volume of the stably stratified air (which contains pollution) is a measure of the ventilation of pollutants from the valley. Thus the rate of emission of pollutants into regional-scale flows above a valley can be related to the decrease of volume of the stably stratified air in which the pollution is trapped. Specifically, the fraction Δf of total pollutant material emitted from a valley segment at a given time step after sunrise is determined as

$$\Delta f_j = \frac{V_{j-1} - V_j}{V_0}, \tag{3}$$

where $V_0 = (h_0 - H_0)w + C(h_0^2 - H_0^2)/2$, the volume of air within the valley inversion per unit length of segment at sunrise, h_0 is the inversion height at sunrise, H_0 is the CBL height at sunrise (10 m), w is the valley floor width, $C = \arctan \alpha_1 + \arctan \alpha_2$, where α_1 and α_2 are the sidewall inclination angles, $V_j = (h_j - H_j)w + C(h_j^2 - H_j^2)/2$, the volume of air within the stable core after j time steps, and $j = 1, 2, 3, \ldots, n$.

The fractions Δf are designated as 'coupling coefficients'. The coupling coefficients must equal unity when summed over the period of inversion destruction. The pollution mass, M_{ij}, which is released from each valley segment i during each time step j, is the coupling coefficient multiplied by the total pollutant mass in a valley segment at sunrise:

$$M_{ij} = M_i \Delta f_j. \tag{4}$$

5. SAMPLE SIMULATIONS

The operation of the parameterization will be illustrated using meteorological and topographical data (Table 1) from two western Colorado valleys, the Eagle and Yampa valleys. Data were collected in these valleys during October 1977 and February 1978, respectively (Whiteman, 1982). For the simulations, a source is assumed to be located in each valley, releasing pollution at a constant rate Q_s. The simulation time step, Δt, is 600 s. Figure 1 shows the variation

Table 1. Inputs to the parameterization for the Eagle and Yampa valleys

		Eagle (16 Oct. 77)	Yampa (23 Feb. 78)	
t_{ss}	(MST)	1720	1750	Sunset (decoupled period begins)
τ_D	(s)	46,800	47,160	Length of decoupled period
t_0	(MST)	0620	0655	Sunrise (coupling starts)
τ	(s)	39,600	39,240	Length of daylight period
w	(m)	1,450	2580	Valley floor width
α_1	(deg)	21	9	Inclination angle of one sidewall
α_2	(deg)	10	16	Inclination angle of other sidewall
A_1	($\mathrm{W\,m^{-2}}$)	906	878	Extraterrestrial solar radiation at solar noon
A_0		0.45	0.19	Fraction of solar radiation to sensible heat
k		0.14	0.00	Fraction of sensible heat for CBL growth
γ	($\mathrm{K\,m^{-1}}$)	0.0269	0.0345	Potential temperature gradient
β	($\mathrm{K\,s^{-1}}$)	0.000083	0.000028	Rate of warming of neutral layer
P	(mb)	768	780	Average air pressure in valley
ρ	($\mathrm{kg\,m^{-3}}$)	0.985	1.035	Average air density in valley
h_0	(m)	650	530	Initial depth of inversion
H_0	(m)	10	10	Initial height of CBL

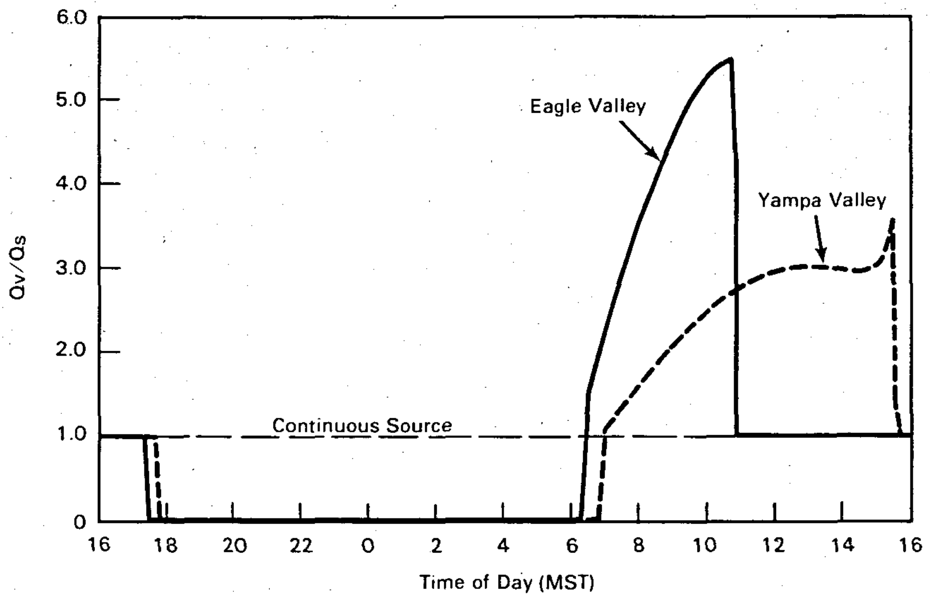

Fig. 1. The pollution release rate to the regional flow from a continuous source located in the Eagle (15–16 October 1977) and Yampa (22–23 February 1978) valleys for a 24-h period. The release rate of pollution trapped in the valley, Q_v, is normalized by the source release rate Q_s.

with time of the pollution release rate Q_v from the Eagle and Yampa valleys, normalized by Q_s for a 24-h period. The valley release rate is determined from Equation (4) such that

$$Q_v = M_{ij}/\Delta t. \tag{5}$$

Each valley is assumed, for this example, to consist of one segment with the characteristics given in Table 1 so that the release rate is representative of the whole valley. The time trace in Fig. 1 begins about 2 h before sunset, showing that pollution sources are releasing directly to the regional flow. After the valley atmosphere becomes decoupled from the regional flow (sunset), the release rate to the regional flow becomes zero. At sunrise, the coupling process begins and pollution trapped in the valley overnight is released to the regional flows during the temperature inversion break-up period. The continuous source is considered to release directly into the regional flow during the entire inversion break-up period beginning at sunrise. After the pollution trapped in the valley is completely vented from the valley, the valley release rate is that of the continuous source.

The dashed line in Fig. 1 labeled 'continuous source' illustrates the assumption commonly made in regional-scale models that cannot resolve valley-scale circulations. All pollution is assumed to be released continuously (day and night), to the regional-scale flows, so that $Q_v/Q_s = 1$. With the use of the valley-scale parameterization, the release rate varies through the course of the day. Pollution released within the valley during the decoupled night-time period is not seen as a source term in the regional-scale model ($Q_v/Q_s = 0$) until the post-sunrise coupling period begins. At this time, the pollutant source is assumed to release directly into the regional-scale flows and the pollution trapped overnight within the valley is dispersed over the length of the coupling period, so that $Q_v/Q_s > 1$ during the coupling period. Note that conservation of pollutant mass requires that the area under the continuous source curve be equal to the areas under the individual valley curves. For the individual valley curves, the mass deficit during the decoupled period is offset by the mass excess during the coupling period. Referring back to section 3, nocturnal pollutant concentration profiles in the valley affect the shape of the coupling period curve, but the total area under the coupling period curve is constrained by the pollutant mass trapped in the valley during the decoupled period.

Figure 1 shows the effect of seasonal variations on pollution release rates [Eagle valley (fall) compared with Yampa valley (winter)]. Pollution trapped in the Yampa valley took almost twice as long to be released to the regional flow as pollution in the Eagle valley for the days presented because the temperature inversion in the Yampa valley took almost twice as long to be destroyed; the ground was snow covered, the inversion was very strong, and the solar input was reduced in winter.

To illustrate the effects of the parameterization on ground-level pollutant concentrations calculated with a regional-scale puff model, the MELSAR model was run for a hypothetical valley system embedded in a flat 500 x 500 km region. The physical and meteorological characteristics of the Eagle valley case given in Table 1 and demonstrated in Fig. 1 were used to define the hypothetical valley system. The simulation started at 1500 h on 15 October 1977 and ended at 1300 h the next day, with the model operating with 1-h time steps.

The valley system was oriented in a north–south direction, as shown by the solid thick line in the various parts of Fig. 2; down-valley was to the south. A continuous source releasing at 1 $g s^{-1}$ was located at the north end of the valley. The regional winds were constant at 3 $m s^{-1}$ from the west, and the stability of the atmosphere above the valley was assumed to be neutral. Sunset occurred at 1700 h and sunrise at 0700 h, for a decoupling period of 11 h. At an average down-valley wind speed of 2 $m s^{-1}$, the pollution would fill approx. 80 km of valley. However, for this simulation the valley transport was limited to approx. 60 km, representing a block to the downvalley flow. The valley system was represented by a total of eight segments; all segments were assumed to have the same physical and meteorological characteristics.

The plume after 2 h is shown in Fig. 2(a). The valley atmosphere is not yet decoupled from the regional flow, and the pollution is being carried in the regional flows. Just after sunset (~1700 h) the valley atmosphere decouples, and the pollution is not released to the regional winds but is contained in the valley until sunrise. In Fig. 2 (b)–(d) is shown the initially released plume being carried off to the east through the night. Just after sunrise (~0700 h), the valley atmosphere begins to couple with the regional winds and the pollution trapped in the valley during the night begins to be released to the regional winds [Fig. 2(e)]. The valley inversion is destroyed near 1100 h, at which time the last of the pollution trapped in the valley is released [Fig. 2(f)]. Figure 2(g) and (h) shows the valley pollution being carried off to the east with the continuous source releasing to the regional winds. For comparison, Fig. 2(i) shows the plume that would result without the valley decoupling–coupling parameterization invoked. The plume would look like this from approx. 0500 h to the end of the simulation [Fig. 2(d)–(h)]. Before this time, the plume would

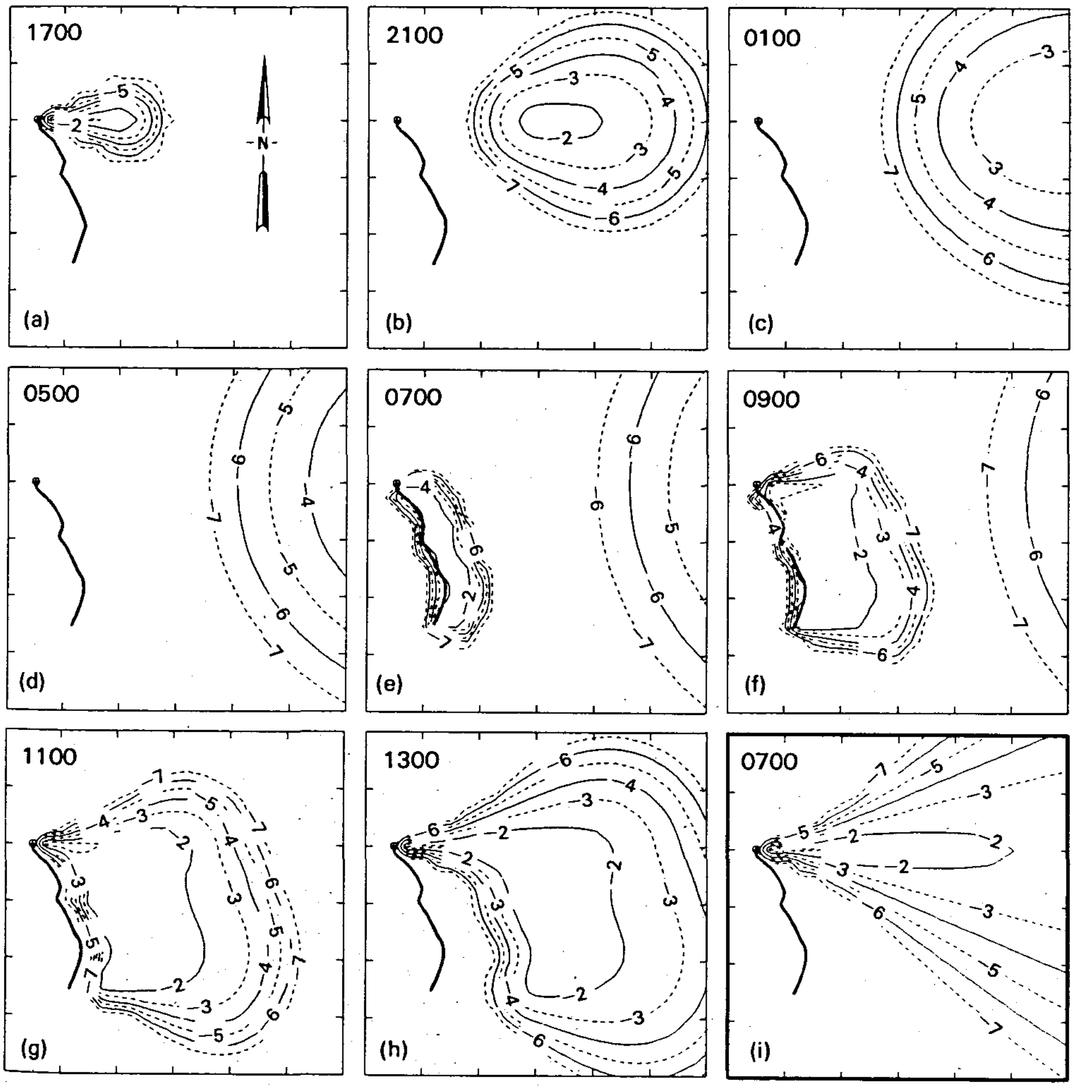

Fig. 2. Results from MELSAR for a continuous point source (1 $g s^{-1}$) located in a hypothetical valley system (thick line). The valley system is assumed to have the characteristics of the Eagle valley (Table 1). The simulation begins at 1500 h on 17 October 1977 and ends at 1300 h the next day. Winds are constant from the west at 3 $m s^{-1}$. Domain shown in each part is 120 km square (each tick mark is 20 km). (a)–(h). Time evolution of ground-level concentrations in which labels on isopleths are exponents of 10. (i). Continuous plume from MELSAR without parameterization invoked.

look exactly as shown in Fig. 2(a), and in Fig. 2(b) and (c) the continuous plume would be connected back to the source.

As mentioned earlier, this decoupling–coupling parameterization is a simplified approach to a rather complex problem. Varying synoptic conditions introduce significant complications. This parameterization also assumes that no pollution remains in the valley atmosphere after the valley inversion is destroyed. In actual cases, some pollution will remain in the well-mixed valley atmosphere after the temperature inversion is destroyed and be released to the regional flow over a period of time.

6. CONCLUSIONS

Pollutants emitted within valleys during the night can be carried down the valleys in locally developed down-valley wind systems. After sunrise, these pollutants may be transported out of the valleys into above-valley regional-scale flows during the post-sunrise 'coupling' period. A simple parameterization has been described for treating the pollution behavior from sources located in valleys during the decoupling–coupling of valley-scale flows with regional-scale flows when the valleys are subgrid scale in the regional model. The parameterization seems appropriate for valleys of sufficient depth to produce confined locally developed flows that routinely become decoupled from regional-scale flows. For continuous sources in such valleys, the pollutant release rate into the regional-scale flows could vary considerably with time. Consequently, it may be important to account for this decoupling–coupling process when modeling the regional transport of pollution in regions where sources are located in valleys and the releases can become trapped in valley flows. The effect on ground-level concentrations of including the parameterization in regional-scale modeling was demonstrated with runs of the regional-scale puff model MELSAR. The area of impact and total exposure to the pollution can be significantly changed by including the parameterization. The degree of effect will decrease when the receptor area of concern is farther away from the source area.

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APPENDIX: INVERSION BREAKUP MODEL

The prediction equations for temperature inversion break-up are as follows (Whiteman and McKee, 1982):

$$\frac{\mathrm{d}H}{\mathrm{d}t}=\frac{\theta}{T}\frac{k}{\rho c_p}\frac{w+HC}{w+HC/2}\frac{A_0A_1}{\gamma H}\sin\frac{\pi}{\tau}(t-t_0) \tag{A1}$$

$$\frac{\mathrm{d}h}{\mathrm{d}t}=-\frac{\theta}{T}\frac{1}{\rho c_p}\frac{[w+hC-k(w+HC)]\,A_0A_1\sin[\pi(t-t_0)/\tau]-\rho c_p(T/\theta)(\beta/2)(h_0-h)[w+(h_0+h)C/2]}{h\gamma(w+hC/2)+(\beta/2)(t-t_0)(w+hC)}, \tag{A2}$$

where h is the depth of the temperature inversion (m), H is the depth of the convective boundary layer (m), θ is potential temperature (K), T is temperature (K), k is the fraction (0–1) of the sensible heat flux used to grow the convective boundary layers, ρ is air density (kg m^{-3}), c_p is the specific heat at constant pressure (1005 J kg^{-2} K^{-1}), w is valley floor width (m), C is the sidewall slope factor ($C=\arctan\alpha_1+\arctan\alpha_2$, where α_1 and α_2 are the sidewall inclination angles), h_0 is the initial depth of the temperature inversion (m), β is the rate of warming in the neutral layer above the valley inversion (K s^{-1}), γ is the potential temperature gradient at sunrise (K m^{-1}), A_0 is the fraction (0–1) of extraterrestrial solar radiation converted to sensible heat flux at the valley surfaces below the inversion top, A_1 is the value of solar radiation at solar noon (W m^{-2}), τ is the length of the daylight period (s), t is time of day (s MST), and t_0 is the time of sunrise (s MST). The value of θ/T is determined from

$$\frac{\theta}{T}=\left(\frac{1000}{P}\right)^{0.286}, \tag{A3}$$

where P is the atmospheric pressure (mb).

Equations (A1) and (A2) are solved numerically to simulate individual episodes of inversion break-up in which the characteristic topographic parameters of the valley (w and C) are obtained from topographic maps and the characteristics of the inversion at sunrise are known from observations of γ

and the initial conditions of h and H. For initial simulations with the model, k may be set to 0.15, a value obtained by fitting Equations (A1) and (A2) to inversion break-up data for Colorado's Eagle valley. Whiteman and McKee (1982) have shown that inversion break-up time is not strongly affected by the choice of a numerical value for k.

The timing of inversion break-up depends critically on the values of several parameters in Equations (A1) and (A2). In particular, it depends on the values of γ and A_0. These parameters can be expected to vary from day to day depending on weather conditions. Since rawinsondes provide the basic data used to drive regional-scale models, we wish to parameterize γ and A_0 based on rawinsonde data collected near the valley. We do this by integrating upward through the morning rawinsonde sounding on a given day to determine the total energy deficit in the surface inversion layer at the rawinsonde site. This value is compared with a mean maximum historical value of the same quantity, and the fraction relating these two is applied to the estimated maximum value of γ for the valley atmosphere (as mentioned) to estimate the value of γ on the day desired.

A_0 is estimated as follows (Allwine and Whiteman, 1985). An integration is performed to determine the thermal energy difference between the morning and late afternoon rawinsonde soundings up to a certain height, which depends on season, and using a method that corrects the integration for advective effects. Second, a time integration is performed on the extraterrestrial solar flux curve for the day of interest to determine the radiation that would have been received between the times of the two rawinsonde soundings. The ratio of these values represents the fraction of extraterrestrial flux converted to sensible heat flux at the rawinsonde station. This fraction is used directly as an estimate of A_0 for the valley.

A theoretical solar radiation model (Whiteman and Allwine, 1987) is used to determine A_1, τ, and t_0. Values for ρ, p and β are estimated for the valley atmosphere from rawinsonde data.