Summary Report for Working Group on:
LINE SYNTHESIS AND ATMOSPHERIC MODELING

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1. INTRODUCTION

The exploration of physical phenomena in the solar atmosphere by means of numerical simulations of atmospheric structure and spectral line formation is an essential complement to increasingly sophisticated observational studies of the Sun. The principal goal of the modeling efforts is to develop diagnostics of physical conditions and processes in 'solar' plasmas.

However, when confronted by the very detailed observations of the solar photosphere and chromosphere, like those reviewed at the Workshop by V. Gaizauskas, F. Deubner, A. Wyller, and others, the atmospheric modeler easily can be overwhelmed by the magnitude of the theoretical effort necessary to accommodate the full range of important phenomena within the framework of numerical simulations. Similarly, the wide variety of important effects revealed by experiments and theoretical studies in atomic physics and spectroscopy can be quite imposing to those concerned with accurate synthesis of spectral line profiles. Accordingly, workers in the fields of atmospheric modeling and line synthesis tend to speak not of their successes, but rather of the obstacles to further progress. The Working Group on Line Synthesis and Modeling focused on four such obstacles: velocity fields, thermal inhomogeneities, geometry, and finite computing resources.

2. VELOCITY FIELDS

Even rudimentary measurements of solar spectra reveal the importance of mass motions. Spectral lines typically exhibit a significant Doppler broadening beyond the thermal component, and oscillatory and stochastic Doppler shifts of features are quite common in the photosphere and chromosphere. In some cases, such as global P-mode oscillations, the velocity fields are a signature of fundamental solar properties (see F. Deubner, these proceedings). In other cases, such as turbulence in the upper chromosphere and lower transition zone, the velocity fields signify the operation of energy transport and dissipation mechanisms. Furthermore, the existence of nonthermal broadening in the solar atmosphere can profoundly affect subsidiary studies, for example the extraction of chemical abundances from mildly saturated absorption (or emission) lines.
2.1 MICRO-, MACRO-, and MESO-TURBULENCE

Unfortunately, it is quite difficult to measure directly the scales and amplitudes of nonthermal velocity fields in the solar atmosphere, at least with the present generation of ground-based instrumentation. Nevertheless, a knowledge of the detailed properties of the nonthermal motions is essential to the atmospheric modeler.

In particular, as demonstrated by the work presented by M. Carlsson at the Workshop, scales of "turbulence" intermediate to those of the microturbulent and macroturbulent limits do not, in general, provide an intermediate line profile shape. Therefore, a proper interpretation of the shape of the Ca II K line emission core, for example, might depend rather sensitively on the detailed character of the nonthermal velocity fields in the chromosphere.

2.2 FREQUENCY REDISTRIBUTION

As another example, the frequency redistribution of scattered radiation in resonance lines depends sensitively on the value of the Voigt parameter, $a_v$, which in turn is inversely proportional to the local Doppler width. Furthermore, the portion of the line profile which is strongly affected by quasi-coherent scattering begins at roughly three Doppler widths from line center. If the coherence scale of the motions is smaller than the photon mean free path between scatterings, the effective Doppler width will be larger than in the case for which the scale of the velocity fields greatly exceeds the scattering length (in the latter case, the appropriate Doppler width is the thermal width.) Therefore, it is essential to know the proper value of $\Delta \lambda_D$ to incorporate into the numerical simulations.

2.2 DYNAMICAL PRESSURE

A third example is the role of small-scale motions in the dynamical pressure balance. In the modeling scheme reviewed at the workshop by E. Avrett, a "turbulent" pressure term, $P_t = 0.5 \rho \xi^2$, is added to the gas pressure term: The additional pressure extends the derived top of the chromosphere to a height compatible with empirical measures of the chromospheric extent from eclipse observations. However, the physical basis for the kinetic pressure term depends in large part on the geometrical scale of the velocity fields, and their degree of isotropy. The quandary concerning the proper way in which to incorporate dynamical effects in static models is resolved to some extent in the explicitly hydrodynamical simulations described by H. Bohn, R. Stein, and others, but in that class of models it is currently impractical to include detailed or elaborate spectral line formation schemes such as in the work of R. Kurucz or E. Avrett and his collaborators (see §5, below).
3. ATMOSPHERIC INHOMOGENEITY

A second important issue raised during the Working Group concerns the spatial and temporal inhomogeneities of the solar atmosphere: It is universally agreed by modelers that the chromosphere is quite inhomogeneous in time and space—a single Hα filtergram movie is sufficiently convincing—but there is a considerable divergence in views concerning the proper strategy to account for such structure in numerical simulations.

3.1 MILD

In the scheme reviewed by E. Avrett, moderate spatial-resolution observations of the Sun in a wide variety of wavelength regions are combined into histograms which indicate the relative frequency of occurrence of different "brightness" levels. Semiempirical model atmospheres then are constructed to match the wavelength behavior of each brightness level. In the 1981 study published by Vernazza, Avrett, and Loeser, six models (A-F) cover a range of brightness of the quiet Sun chromosphere from "inactive" to "moderately active". Because the models are derived from a smoothly varying distribution of brightness levels, the thermal structures of the individual components are quite similar to one another, and the degree of inhomogeneity is comparatively mild. Given the range of thermal structure models, in principle one can simulate the spatial averaging that occurs on the solar surface by weighting each of the model profiles by the frequency of occurrence. In this manner, Vernazza, Avrett, and Loeser established that the explicitly-averaged profiles of important chromospheric diagnostics like Ca II K and Mg II k were very similar to profiles calculated for the single, mean chromospheric temperature distribution (their model "C"). The authors' results suggest that the effects of spatial averaging are only of second-order importance in interpretations of solar line profiles.

3.2 EXTREME

An alternative view of solar inhomogeneities was presented by T. Ayres in a discussion of observational studies by Ayres and Testerman, published in 1981, and more recent work by Ayres, Testerman, and Brault (in preparation). The two studies have focused on the 4.6μm fundamental vibration-rotation bands of solar carbon monoxide. The CO bands are optically thick at the base of the chromospheric temperature inversion, and are useful diagnostics of the T_min region because the vibration-rotation transitions are thought to be formed in LTE. However, the cores of the strongest of the CO lines are not centrally reversed in the quiet Sun or in active regions (Ca II K plages), contrary to the predictions of conventional chromospheric models. Instead, the CO features exhibit "cool cores" which indicate the presence of low-temperature material (T < 4000 K) at, and above, the heights where existing models place the temperature inversion (T_min ≠ 4500 K). The explanation for the cool cores in the CO bands invokes a highly inhomogeneous, two-component model, in which a pervasive, cool photosphere is interrupted by small-scale chromospheric "hot spots": The distinction between quiet and active regions is the fractional
area covered by the hot spots; small in the former, but larger in the latter. In the situation of the thermally "bifurcated" atmosphere, the spatially-averaged profiles of Ca II K and Mg II k bear no direct relation to the very distinct thermal structures of the two components: A mean model derived from spatially-averaged spectra will provide only a misleading picture of the true thermal structure of the atmosphere.

While the "mild" and "extreme" scenarios propose very different views of the spatial inhomogeneity of the solar chromosphere, it is difficult to decide conclusively at the present time which is the more appropriate: Observations of the solar surface with sufficient spatial resolution and temporal coherence to determine directly the geometrical scales of "activity" must be undertaken from space, while the thermal bifurcation model itself rests on a simple (i.e. LTE) interpretation of only a single spectral diagnostic. Clearly, additional observational and theoretical effort must be devoted to answer the critical question of the degree of thermal inhomogeneity in the solar chromosphere.

3.3 HYBRID

Indeed, the possibility was raised at the Workshop that a hybrid model atmosphere with some of the characteristics of the "mild" and "extreme" classes of inhomogeneities might be able to reproduce the conflicting observations. In particular, F. Kezer described a radiative equilibrium simulation incorporating CO cooling which exhibited a sharp temperature drop at and above the conventional height of the $T_{\text{min}}$, but which also developed a chromospheric temperature inversion at higher levels. On the one hand, the sharp temperature drop—the "cold pit"—would be quite visible in the CO lines since the molecular absorption is strongly weighted to cool temperatures; but it would be nearly invisible in the inner wings of the Ca II and Mg II features owing to the long range of the partial-coherent-scattering source functions, and the exponential weighting of the ultraviolet emissivity to higher temperatures (Wein limit of the Planck function). On the other hand, the temperature inversion in higher layers would be visible in the Ca II and Mg II lines; but it would not be seen in CO, because the molecular bands are optically thin at those altitudes. Clearly, such a hybrid model should be investigated as an alternative to the extreme-inhomogeneity scenario.

4. GEOMETRY

A third area which received considerable attention during the discussions of the Working Group was the question of geometry, particularly the vertical spreading of magnetic flux tubes (so-called "canopies"). The geometry of structures manifests itself in two important ways.

4.1 OVERLAP/SHADOWING

Firstly, the existence of canopies implies that the line of sight to the surface might pass through material of very different excitation which is not arrayed in the conventional manner, namely a monotonically outward increasing
temperature (above the $T_{\text{min}}$, at least). If one is examining a diagnostic that has significant contributions from distinct regions along the line of sight, a knowledge of the geometry is essential for a proper interpretation of that diagnostic. If two spectral features of interest are formed preferentially in different structures, then a joint homogeneous analysis of the emergent intensities could produce a very misleading physical picture. Conversely, a careful selection of complementary diagnostics might provide one with the empirical distribution of temperature along several lines of sight, from which the geometrical properties of a structure could be recovered.

4.2 PHOTON DIFFUSION

Secondly, certain classes of geometries, particularly very thin tubes, might be misinterpreted in conventional analyses of important diagnostics like Ly$\alpha$, Mg II k, and Ca II K which have large "thermalization" lengths. In particular, photons produced in a hot, thin magnetic flux tube could scatter horizontally in the cooler external medium for distances several times larger than the diameter of the filament, and then be scattered vertically into the line of sight. Therefore, even in spatially resolved images of the highest quality, a structure might appear to be significantly broader in Ca II light, owing to photon diffusion, than the actual physical extent of the high-excitation region. In that situation, one must be prepared to investigate alternative diagnostics with significantly different thermalization properties.

5. COMPUTING RESOURCES

A final topic of discussion of the Working Group were the constraints that often are imposed by limitations in the hardware and software which modelers have at their disposal to undertake numerical simulations. Historically, limitations in computing resources have resulted in simulations that stress a particular aspect of a model-atmosphere/line-formation system, while invoking simplifications in what are perceived to be less essential aspects of the problem. Examples of that duality from the Workshop include: The study of intermediate scale velocity fields by M. Carlsson and G. Scharmer, in which elaborate simulations of the effects of stochastic velocity fields of different geometrical scale lengths were undertaken for a simple treatment of the frequency-redistribution process—non-coherent scattering—and in a fixed, one-dimensional thermal model; the study of resonance polarization in the Ca II K line by G. Saliba, in which a complex, quantum mechanical treatment of the polarization of the scattering process was calculated for a comparatively simple atmospheric model; and the hydrodynamic models of the chromosphere reported by H. Bohn and R. Stein, in which a detailed simulation of dynamical processes was coupled with a schematic treatment of the radiative equilibrium, namely a quasi-grey opacity.

With enough patience and attention to detail, it is possible to stretch the limitations imposed by finite computing resources. An example is the elaborate set of semi-empirical model simulations which have been developed by E. Avrett and collaborators, and reviewed at the Workshop. The simulations incorporate very detailed atomic models and statistical equilibrium calcula-
tions, with special attention paid to the ionization balance and the formation of resonance lines including partial-frequency redistribution. A range of thermal models were constructed to match distributions of line and continuum intensities based on a broad variety of moderate spatial resolution observations (see §3.1, above). Such models are very useful for studying the effects of averaging on observations of low spatial resolution (e.g., stellar spectra), as well as on the derivation of radiative cooling rates in the chromosphere. Nevertheless, by necessity the semiempirical models incorporate only a rudimentary treatment of chromospheric velocity fields.

Another example of stretching the limits imposed by finite computing resources, are the elaborate radiative equilibrium and spectrum synthesis simulations undertaken by R. Kurucz. In these calculations, great attention is paid to the treatment of the literally millions of atomic, molecular, and ionic transitions that contribute to the overall opacity of the solar (and stellar) atmosphere. Such calculations have demonstrated their value in a number of applications, for example in the study of the effects of weak blends on Zeeman-sensitive absorption lines in late-type stellar spectra, whose anomalous broadening has been interpreted as evidence for surface magnetic fields. However, owing to the exceedingly detailed treatment of line blanketing in the radiative equilibrium simulations, the statistical equilibrium must be undertaken in LTE, and the line profile shapes must be calculated with the assumption of noncoherent scattering.

A final remark: The elaborate, but narrowly focused, class of simulations described in the preceding examples play an important, complementary role to more general numerical studies; particularly when the former point to appropriate approximation schemes, like opacity tables or analytical interpolation formulae, which can be employed in the latter.

6. CONCLUSIONS

Many of the impediments to further progress in the field of atmospheric modeling and line synthesis result from our present inability to fully resolve the spatial and temporal behavior of phenomena and processes in the solar atmosphere. This is a somewhat disturbing situation, particularly with regard to stellar observations for which solar-class spatial resolution cannot be obtained with present technology. Therefore, the Sun offers us essentially the only laboratory for the detailed study of the subtleties of atmospheric structure and line formation among late-type stars.

In order to solve the current problems in the field, we must obtain high-quality ultraviolet, optical, and infrared observations of the Sun from space (i.e., using SOT and related experiments), and exploit "new" diagnostics that provide complementary information from that of the traditional diagnostics. An example is the millimeter and submillimeter band (see L. Cram, these proceedings), particularly as observed during solar eclipses, where the moving limb of the moon provides the opportunity to obtain fine-scale thermal cross-sections of the solar chromosphere. High spatial resolution and high temporal resolution measurements of traditional diagnostics, like Ca II K and Hα, can help address the question of the geometrical scales of atmospheric velocity fields and short-lived acoustic disturbances. Finally, concerted efforts in the areas of laboratory and theoretical atomic physics are essential to pro-
vide accurate cross-sections for the processes modeled in line formation simulations.

ACKNOWLEDGEMENTS

I thank the participants of the Working Group for the stimulating discussions during our meetings. This work was supported by the National Science Foundation through grant AST 8203450 to the University of Colorado.