Modification of CRTM Surface Emissivity Adjoint Codes to Reconcile the Applications in DA QC & 1DVAR Retrieval

1. Prompt Question

This CRTM code modification and improvement effort was prompted by Mingjing's question on the negative surface emissivity Jacobin (adjoint) value where the CRTM RTV%Scattering_RT is true. The following is mingjing's original email message to Mark on October 24:

I'm running GSI for FV3GFS using all 5 hydrometers (cloud liquid water, cloud ice, rain, snow and graupel) as control variables. So the water content of all five hydrometeors are the input to CRTM. I found that when including all five hydrometeors, the surface emissivity sensitivity has been change a lot. Please see the attached figures. I'm comparing ***two experiments.***

QLQI: *only include cloud liquid water and cloud ice*

ALLQ: *include all five hydrometeors*

You can see that the surface emissivity sensitivity of the QLQI experiment are all positive. But for ALLQ experiment, most of the locations are negative.

After digging into the CRTM code (I'm using version 2.3.0), I found that in the subroutine ***Assign_Common_Output_AD*** *in* ***Common_RTSolution.f90****, the following part of the code ran differently for the two experiments.*

```
IF( RTV%Scattering_RT ) THEN
  User_Emissivity_AD = ZERO
  IF( RTV%Diffuse_Surface) THEN
    DO i = nZ, 1, -1
      User_Emissivity_AD = User_Emissivity_AD - &
        (SUM(SfcOptics_AD%Reflectivity(1:nZ,1,i,1))*SfcOptics%Weight(i))
    END DO
  ELSE ! Specular surface
    DO i = nZ, 1, -1
      User_Emissivity_AD = User_Emissivity_AD - SfcOptics_AD%Reflectivity(i,1,i,1)
    END DO
  END IF
!     Direct_Reflectivity_AD = SUM(SfcOptics_AD%Direct_Reflectivity(1:nZ,1))
!     SfcOptics_AD%Direct_Reflectivity(1,1) = SfcOptics_AD%Direct_Reflectivity(1,1) +
!                                  (Direct_Reflectivity_AD/PI)
  RTSolution_AD%Surface_Emissivity = User_Emissivity_AD
ELSE
  RTSolution_AD%Surface_Emissivity = SfcOptics_AD%Emissivity(SfcOptics_AD%Index_Sat_Ang,1) - &
                                     SfcOptics_AD%Reflectivity(1,1,1,1)
END IF
```

For the QLQI experiment, it never ran into the red block of the code, which means RTV%Scattering_RT is always False. It is because CRTM_Include_Scattering(AtmOptics) is *always False or MAXVAL(atmoptics%Single_Scatter_Albedo) is never greater than the single scatter albedo threshold.*

While for the ALLQ experiment, a lot of data point fall into the bold red block (Only AMSUA and ATMS are assimilated in all-sky mode). As you can see, User_Emissivity_AD is set to zero at the beginning, SfcOptics_AD%Reflectivity(i,1,i,1) is always positive. As long as CRTM ran into the red block, the emissivity sensitivity is always negative.

The positive jacobin of surface emissivity makes sense to me. Do you think this is an error in CRTM code?

Mingjing also attached her case study results in her message to demonstrate her question. Shown in Figure 1 are the different surface emissivity Jacobins of CRTM REL 2.3.0 in ALAI and ALLQ at NOAA AMSUA Ch2 from Mingjing's case study. It may be easily seen that the surface emissivity Jacobin is always positive in the QLQI case while in the ALLQ case, it becomes negative almost everywhere. Since Tb≈ε*Ts in MW bands, one would respect a positive surface emissivity Jacobian (adjoint) in any case.

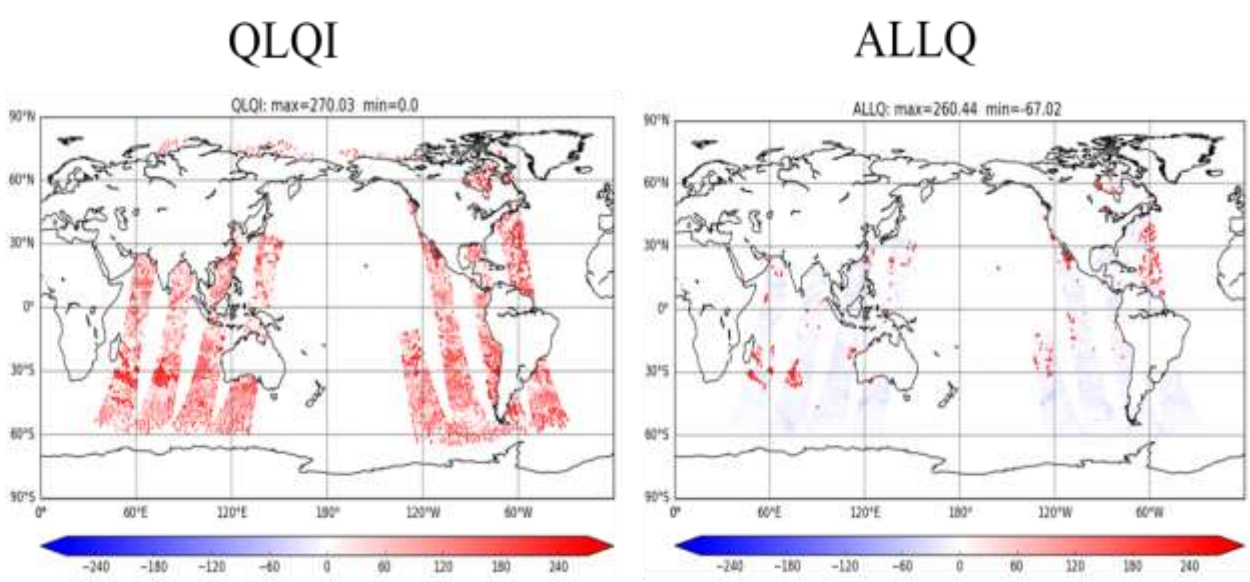


Figure 1. The different surface emissivity Jacobins of CRTM REL 2.3.0 in Scattering and Non-Scattering conditions

Emily also reported this similar issue even at an earlier time when she performed comparative analysis with CRTM and RTTOV. Shown in Figure 2 is Emily's analysis. CRTM surface emissivity Jacobian did become negative in scattering condition while RTTOV has positive surface emissivity Jacobian in both non-scattering and scattering conditions.

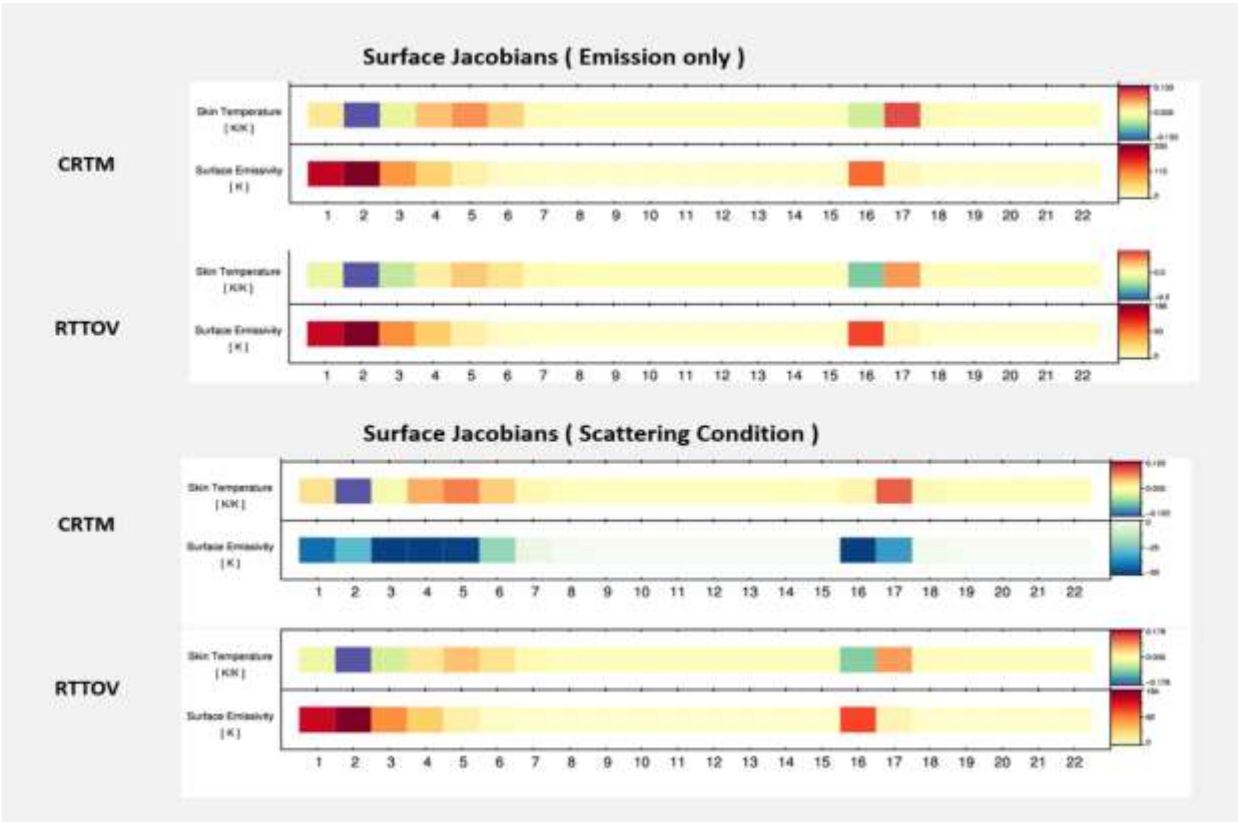


Figure 2. Comparison of Surface emissivity Jacobins of CRTM REL 2.3.0 and RTTOV in Scattering and Non-Scattering conditions

2. Analysis of the Question

Note that the negative surface emissivity Jacobian issue identified in both Emily's and Mingjing's case studies were all of MW ocean surface, where surface emissivity is calculated with FASTEM model. In general, the TOA Tb will become less and less sensitive to surface while the atmosphere is covered by more and more clouds. So one would expect that the surface emissivity Jacobian approaches zero when the cloud amount increases to certain amount. To better understand if the current CRTM has this basic feature, we performed the following single-profile off-line CRTM testing, where different rain cloud profiles are set so that we may easily analyze the basic asymptotic feature of surface emissivity Jacobian in response to the change of the cloud amount. Shown in Table 1 is the surface emissivity Jacobian with unit Tb difference of ATMS Surface channels over ocean. In the testing, all the CRTM inputs are fixed except for different rain cloud water content profiles are preset to mimic different cloud water loads. There are three main features:

1) In clear-sky case, the surface emissivity Jacobian is always positive, which is consistent with what were found in Minjing's and Emily's analyses. The surface emissivity Jacobian varies with respect to frequency and view angles. In general, the surface emissivity Jacobian becomes smaller at higher frequency channel and larger view angle. But the angular dependency becomes less significant in more cloudy cases.
2) The surface emissivity Jacobian becomes negative once rain cloud appears where CRTM scattering mechanism is turned on. And the surface emissivity Jacobian do approach zero when the rain cloud amount increase to certain amount.
3) Nevertheless, the absolute value of the negative surface emissivity Jacobian does not monotonically decrease to zero, it creases first then decreases to zero, which is hard to understand in Physics.

Table 1. Surface emissivity Jacobian with unit Tb difference of ATMS Surface channels over ocean

Nadir

Cloud Water Content	23GHz	31GHz	50GHz	51GHz
0.0	237.284	248.684	116.841	66.713
0.5	-60.424	-64.004	-34.379	-25.525
1.0	-62.786	-49.691	-9.867	-6.62
1.5	-52.851	-30.789	-2.558	-1.599
2.0	-40.707	-17.579	-0.648	-0.38
2.5	-29.929	-9.675	-0.163	-0.09
3.0	-21.418	-5.23	-0.041	-0.021
3.5	-15.074	-2.801	-0.01	-0.005
4.0	-10.497	-1.493	-0.003	-0.001
4.5	-7.259	-0.794	-0.001	0
5.0	-4.996	-0.422	0	0
5.5	-3.428	-0.224	0	0
6.0	-2.348	-0.119	0	0
6.5	-1.605	-0.063	0	0
7.0	-1.097	-0.033	0	0
7.5	-0.749	-0.018	0	0

35°

Cloud Water Content	23GHz	31GHz	50GHz	51GHz
0.0	229.29	242.629	95.824	48.27
0.5	-63.372	-62.662	-24.32	-16.414
1.0	-62.786	-49.691	-9.867	-6.62
1.5	-52.851	-30.789	-2.558	-1.599
2.0	-40.707	-17.579	-0.648	-0.38
2.5	-29.929	-9.675	-0.163	-0.09
3.0	-21.418	-5.23	-0.041	-0.021
3.5	-15.074	-2.801	-0.01	-0.005
4.0	-10.497	-1.493	-0.003	-0.001
4.5	-7.259	-0.794	-0.001	0
5.0	-4.996	-0.422	0	0
5.5	-3.428	-0.224	0	0
6.0	-2.348	-0.119	0	0
6.5	-1.605	-0.063	0	0
7.0	-1.097	-0.033	0	0
7.5	-0.749	-0.018	0	0

70°

Cloud Water Content	23GHz	31GHz	50GHz	51GHz
0.0	176.326	201.043	22.65	4.854
0.5	-49.239	-29.332	-1.2	-0.425
1.0	-62.786	-49.691	-9.867	-6.62
1.5	-52.851	-30.789	-2.558	-1.599
2.0	-40.707	-17.579	-0.648	-0.38
2.5	-29.929	-9.675	-0.163	-0.09
3.0	-21.418	-5.23	-0.041	-0.021
3.5	-15.074	-2.801	-0.01	-0.005
4.0	-10.497	-1.493	-0.003	-0.001
4.5	-7.259	-0.794	-0.001	0
5.0	-4.996	-0.422	0	0
5.5	-3.428	-0.224	0	0
6.0	-2.348	-0.119	0	0
6.5	-1.605	-0.063	0	0
7.0	-1.097	-0.033	0	0
7.5	-0.749	-0.018	0	0

Obviously, CRTM does have proper mechanism to reflect the TOA Tb sensitivity to surface emissivity. All the problem is the negative surface emissivity Jacobian when the CRTM scattering is turned on.

To better understand the problem, we performed a thorough check of all the related CRTM codes, particularly the coherency among the related forward, tangent and adjoint modules.

Shown in Figure 3 is the related CRTM codes in the forward mode. There is two major IF condition blocks: one (yellowed) separates the Computed-emissivity (or model simulated) from the Non-computed (user-defined, or the direct emissivity input from user); the other is the Scattering and Non-Scattering WHITHIN the Non-Computed block. In general, Non-Computed emissivity will be used in variational emissivity retrieval, e.g., MiRS. Shown in Figure 4 is the corresponding adjoint-mode codes. One may easily identify the inconsistency in the general conditional control blocks. There is no control to separate the Computed and Non-computed blocks. In this case, the surface emissivity Jacobian of Non-computed case is also taken as the output for the case of the Computed (model calculated), which is basically wrong in physics. The model calculated emissivity and reflectivity follows the intrinsic physical constraints, which is particularly essential for the diffusive surfaces where the emissivity is actually a bulk effective physical quantity. By contrast, the surface emissivity Jacobian is totally based on some simple assumption between the surface reflectivity and emissivity in the Non-computed (user-defined emissivity) case.

Over ocean, surface emissivity is calculated from FASTEM in general applications, which is just the case in Mingjing's and Emily's studies. But the surface emissivity Jacobian in their studies were actually from the Non-computed case in the current CRTM release. So in order to fix the problem, we need to modify the CRTM codes to output the surface emissivity Jacobian in the model-calculated condition.

```
! ----------------------------------
! Populate the SfcOptics structure
! ----------------------------------
IF ( SfcOptics%Compute ) THEN
  Error_Status = CRTM_Compute_SfcOptics( &
           Surface    , & ! Input
           GeometryInfo, & ! Input
           SensorIndex , & ! Input
           ChannelIndex, & ! Input
           SfcOptics  , & ! In/Output
           RTV%SOV     ) ! Internal variable output
  IF ( Error_Status /= SUCCESS ) THEN
    WRITE( Message,'("Error computing SfcOptics for ",a," channel ",i0)' ) &
         TRIM(SC(SensorIndex)%Sensor_Id), &
         SC(SensorIndex)%Sensor_Channel(ChannelIndex)
    CALL Display_Message( ROUTINE_NAME, TRIM(Message), Error_Status )
    RETURN
  END IF
```

```
ELSE

 IF( RTV%Scattering_RT ) THEN
  ! Replicate the user emissivity for all angles
  SfcOptics%Reflectivity = ZERO
  User_Emissivity = SfcOptics%Emissivity(1,1)
  SfcOptics%Emissivity(1,1) = ZERO
  Direct_Reflectivity = SfcOptics%Direct_Reflectivity(1,1)/PI
  SfcOptics%Emissivity(1:nZ,1) = User_Emissivity
  ! Replicate the user reflectivities for all angles
  SfcOptics%Direct_Reflectivity(1:nZ,1) = Direct_Reflectivity

  IF( RTV%Diffuse_Surface) THEN
   DO i = 1, nZ
    SfcOptics%Reflectivity(1:nZ, 1, i, 1) = &
   (ONE-SfcOptics%Emissivity(i,1))*SfcOptics%Weight(i)
   END DO
  ELSE ! Specular surface
   DO i = 1, nZ
    SfcOptics%Reflectivity(i, 1, i, 1) = (ONE-SfcOptics%Emissivity(i,1))
   END DO
  END IF

 ELSE
  User_Emissivity = SfcOptics%Emissivity(1,1)
  SfcOptics%Emissivity( SfcOptics%Index_Sat_Ang,1 ) = User_Emissivity
  SfcOptics%Reflectivity(1,1,1,1) = ONE - User_Emissivity
 END IF

END IF
```

Figure 3. The related forward CRTM codes in question

```
IF( RTV%Scattering_RT ) THEN
  User_Emissivity_AD = ZERO

  IF( RTV%Diffuse_Surface) THEN
   DO i = nZ, 1, -1
    User_Emissivity_AD = User_Emissivity_AD - &
     (SUM(SfcOptics_AD%Reflectivity(1:nZ,1,i,1))*SfcOptics%Weight(i))
   END DO
  ELSE ! Specular surface
   DO i = nZ, 1, -1
    User_Emissivity_AD = User_Emissivity_AD - SfcOptics_AD%Reflectivity(i,1,i,1)
   END DO
  END IF

  RTSolution_AD%Surface_Emissivity = User_Emissivity_AD
ELSE
  RTSolution_AD%Surface_Emissivity = &
      SfcOptics_AD%Emissivity(SfcOptics_AD%Index_Sat_Ang,1) - &
                 SfcOptics_AD%Reflectivity(1,1,1,1)
END IF
```

```
IF ( SfcOptics%Compute ) THEN
  Error_Status = CRTM_Compute_SfcOptics_AD( &
          Surface    , & ! Input
          SfcOptics  , & ! Input
          SfcOptics_AD, & ! Input
          GeometryInfo, & ! Input
          SensorIndex , & ! Input
          ChannelIndex, & ! Input
          Surface_AD  , & ! In/Output
          RTV%SOV     ) ! Internal variable input
  IF ( Error_Status /= SUCCESS ) THEN
    WRITE( Message,'("Error computing SfcOptics_AD for ",a," channel ",i0)' ) &
        TRIM(SC(SensorIndex)%Sensor_Id), &
        SC(SensorIndex)%Sensor_Channel(ChannelIndex)
    CALL Display_Message( ROUTINE_NAME, TRIM(Message), Error_Status )
    RETURN
  END IF
END IF
```

Figure 4. The related adjoint CRTM codes in question

3. Modification of the CRTM Codes

Figure 5 shows the code changes we made to reconcile the two different applications. Actually, to ensure the correctness, we performed several tests before we came up with the current changes:

1) To ensure the surface emissivity Jacobin retained in SfcOptics_AD is the same as that from the temporal (working) RTSolution (RTV_AD) and the final RTSolution_AD, especially the surface emissivity Jacobin at the satellite view angle.
2) To ensure the consistency among the Forward, Tangent linear and Adjoint modules.
3) To ensure that the current changes wouldn't affect the previous Non-Computed applications, particularly the operational MiRS applications.
4) To ensure the correctness of the surface emissivity Jacobin in model-computed condition, that is, we should have positive surface emissivity Jacobin, and the positive surface emissivity Jacobin will approaches to zero when the atmospheric cloud increase to certain amount.

```
IF ( .NOT. SfcOptics%Compute ) THEN

 IF( RTV%Scattering_RT ) THEN
   User_Emissivity_AD = ZERO

   IF( RTV%Diffuse_Surface) THEN
    DO i = nZ, 1, -1
     User_Emissivity_AD = User_Emissivity_AD - &
      (SUM(SfcOptics_AD%Reflectivity(1:nZ,1,i,1))*SfcOptics%Weight(i))
    END DO
   ELSE ! Specular surface
    DO i = nZ, 1, -1
     User_Emissivity_AD = User_Emissivity_AD - SfcOptics_AD%Reflectivity(i,1,i,1)
    END DO
   END IF

   RTSolution_AD%Surface_Emissivity = User_Emissivity_AD
 ELSE
   RTSolution_AD%Surface_Emissivity = &
        SfcOptics_AD%Emissivity(SfcOptics_AD%Index_Sat_Ang,1) - &
                     SfcOptics_AD%Reflectivity(1,1,1,1)
 END IF
```

```
ELSE
 RTSolution_AD%Surface_Emissivity = &
    SfcOptics_AD%Emissivity(SfcOptics_AD%Index_Sat_Ang,1)
 IF ( SfcOptics%Compute ) THEN
   Error_Status = CRTM_Compute_SfcOptics_AD( &
            Surface    , & ! Input
            SfcOptics   , & ! Input
            SfcOptics_AD, & ! Input
            GeometryInfo, & ! Input
            SensorIndex , & ! Input
            ChannelIndex, & ! Input
            Surface_AD  , & ! In/Output
            RTV%SOV      ) ! Internal variable input
   IF ( Error_Status /= SUCCESS ) THEN
    WRITE( Message,'("Error computing SfcOptics_AD for ",a," channel ",i0)' )
&
      TRIM(SC(SensorIndex)%Sensor_Id), &
      SC(SensorIndex)%Sensor_Channel(ChannelIndex)
    CALL Display_Message( ROUTINE_NAME, TRIM(Message),
Error_Status )
    RETURN
   END IF
  END IF

 END IF
```

Figure 5. The Fixed adjoint CRTM codes in question

4. Testing Results with the Modified CRTM

The following Section summaries the testing results by Ming (CRTM), Mingjing & Emily (DA) and Chris (MiRS). All the testing results indicate that the current code changes do fix the issue reported by Mingjing and Emily and will not affect the current MiRS operational applications.

1) CRTM Single-profile Offline Testing (Table 2)
   This testing is similar to that shown in Table 1. In comparison with Table 1, one may find that all the surface emissivity Jacobian become positive. And as one may expect, the surface emissivity Jacobian also has proper asymptotic features as the atmospheric cloud increases, which indicates that the TOA Tb becomes less sensitive to the surface emissivity.

Table 2. Surface emissivity Jacobian with unit Tb difference with Fixed CRTM codes

Nadir

Cloud Water Content	23GHz	31GHz	50GHz	51GHz
0.0	257.839	263.932	177.002	131.255
0.5	175.736	139.894	44.458	31.041
1.0	119.777	74.149	11.166	7.341
1.5	81.637	39.302	2.805	1.736
2.0	55.641	20.831	0.704	0.411
2.5	37.924	11.042	0.177	0.097
3.0	25.848	5.852	0.044	0.023
3.5	17.617	3.102	0.011	0.005
4.0	12.007	1.644	0.003	0.001
4.5	8.184	0.871	0.001	0
5.0	5.578	0.462	0	0
5.5	3.802	0.245	0	0
6.0	2.591	0.13	0	0
6.5	1.766	0.069	0	0
7.0	1.204	0.036	0	0
7.5	0.82	0.019	0	0

35°

Cloud Water Content	23GHz	31GHz	50GHz	51GHz
0.0	253.31	260.575	159.321	110.277
0.5	158.638	120.053	29.496	18.97
1.0	119.777	74.149	11.166	7.341
1.5	81.637	39.302	2.805	1.736
2.0	55.641	20.831	0.704	0.411
2.5	37.924	11.042	0.177	0.097
3.0	25.848	5.852	0.044	0.023
3.5	17.617	3.102	0.011	0.005
4.0	12.007	1.644	0.003	0.001
4.5	8.184	0.871	0.001	0
5.0	5.578	0.462	0	0
5.5	3.802	0.245	0	0
6.0	2.591	0.13	0	0
6.5	1.766	0.069	0	0
7.0	1.204	0.036	0	0
7.5	0.82	0.019	0	0

70°

Cloud Water Content	23GHz	31GHz	50GHz	51GHz
0.0	221.079	236.286	73.062	30.418
0.5	72.072	36.929	1.286	0.449
1.0	119.777	74.149	11.166	7.341
1.5	81.637	39.302	2.805	1.736
2.0	55.641	20.831	0.704	0.411
2.5	37.924	11.042	0.177	0.097
3.0	25.848	5.852	0.044	0.023
3.5	17.617	3.102	0.011	0.005
4.0	12.007	1.644	0.003	0.001
4.5	8.184	0.871	0.001	0
5.0	5.578	0.462	0	0
5.5	3.802	0.245	0	0
6.0	2.591	0.13	0	0
6.5	1.766	0.069	0	0
7.0	1.204	0.036	0	0
7.5	0.82	0.019	0	0

2) Mingjing's testing
   Figure 6 is similar to Figure 1, but with the modified CRTM. As shown in Figure 6, the surface emissivity Jacobian now becomes positive in ALLQ case, but it is hard to tell the sensitivity difference between non-scattering (QLQI) and scattering ALLQ due to the coloring scales.

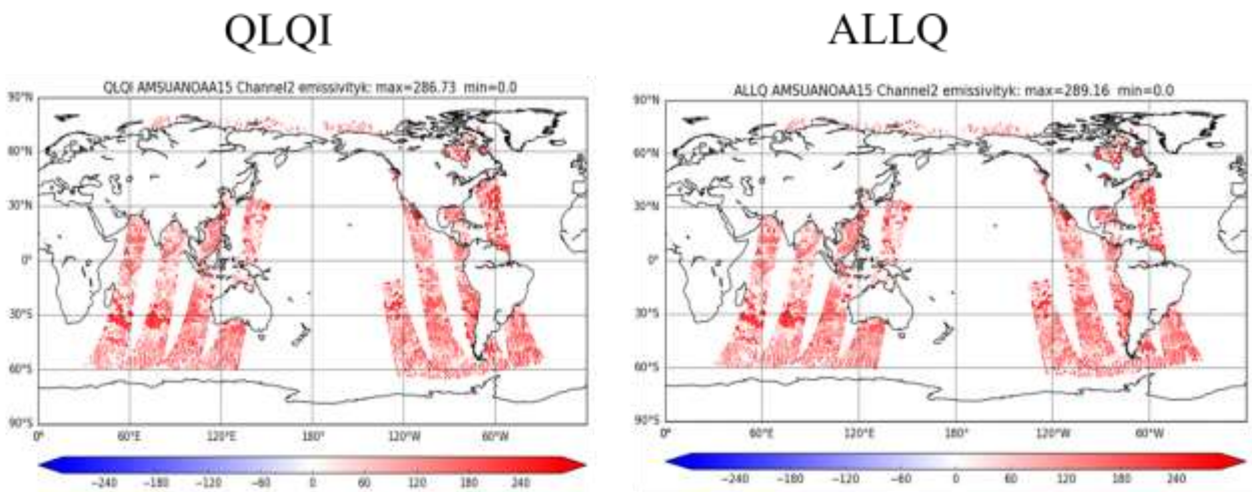
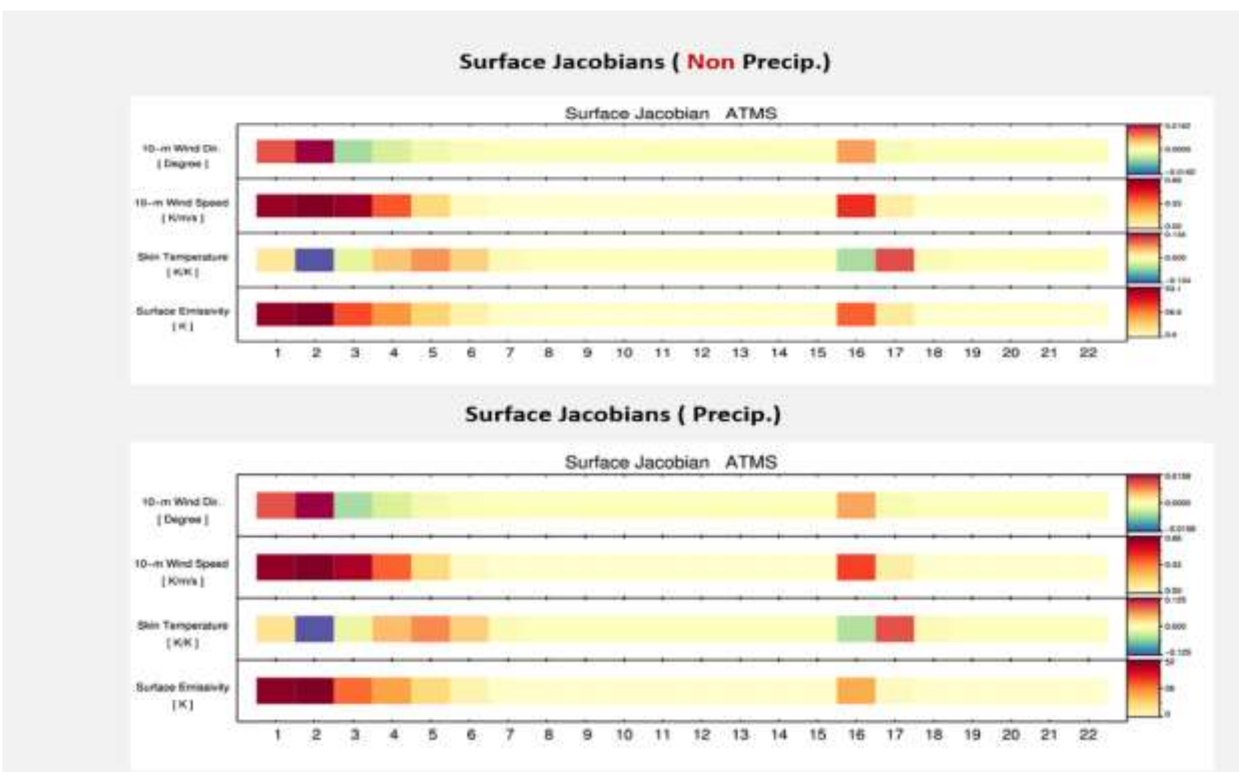


Figure 6. Surface emissivity Jacobins of CRTM REL 2.3.0 in Scattering and Non-Scattering conditions with Fixed CRTM codes

3) Emily's Testing

   Figure 7 is similar to Figure 2 but with the modified CRTM. It may be seen that issue shown in Figure 2 has been solved.



4) Chris's Testing

Chris performed very comprehensive testing to ensure that the current CRTM code changes wouldn't affect the existing MiRS quality. The operational MiRS still uses CRTM REL 2.1.1, and more importantly, MiRS CRTM has different assumptions for ocean and non-ocean surfaces. Ocean surface is assumed specular and all other non-ocean surfaces are assumed to be diffusive.

Figure 8 shows the testing results with the operational MiRS where the non-ocean surfaces are diffusive, and ocean surface is assumed to be specular. The modified CRTM may produce results identical to the operational MiRS. Chris also tested the case where all the surfaces are assumed to specular. The results are shown in Figure 9. It may be seen that the modified CRTM didn't alter the MiRS results either in this case.

Here is the summary by Chris.

Tests Run:

- OPER (CRTM 2.1.1 with 2014 modification , diffuse reflection for non-ocean surfaces)
- TEST 1 (CRTM 2.1.1 with Mark's 2018 modification)
- TEST 2 (CRTM 2.1.1 with Mark's 2018 modification+allSfc=Specular)
- TEST 3 (CRTM 2.1.1 with Ming's 2018 modification)
- TEST 4 (CRTM 2.1.1 with Ming's 2018 modification+allSfc=Specular)

Results indicated:

1. Ming's modification and assuming diffuse reflection for non-ocean surfaces (TEST 3) gave IDENTICAL results to current MiRS operational (OPER: CRTM 2.1.1 with 2014 modification from Dave Groff, assumes diffuse reflection for non-ocean surfaces)
2. For both Mark's and Ming's modification, assuming specular reflection for all surfaces (TEST 2, TEST 4) gave better results than assuming diffuse reflection for non-ocean surfaces. (TEST 1, TEST 3)
3. When assuming specular reflection for all surfaces, BOTH Mark's and Ming's modification gave IDENTICAL results. (TEST 2, TEST 4)
4. The modifications assuming specular reflection for all surfaces (TEST 2, TEST 4) generally yielded improved results compared to the current operational MiRS. Scan dependence in Tskin over snow and ice is reduced (compared to ECMWF), and the overall bias in Tskin is reduced over snow.
5. Note that in comparing retrieved emissivity to "analytic" emissivity over non-ocean, the analytic emissivity is computed using a specular assumption, making comparisons with retrievals that assume diffuse reflection ambiguous.

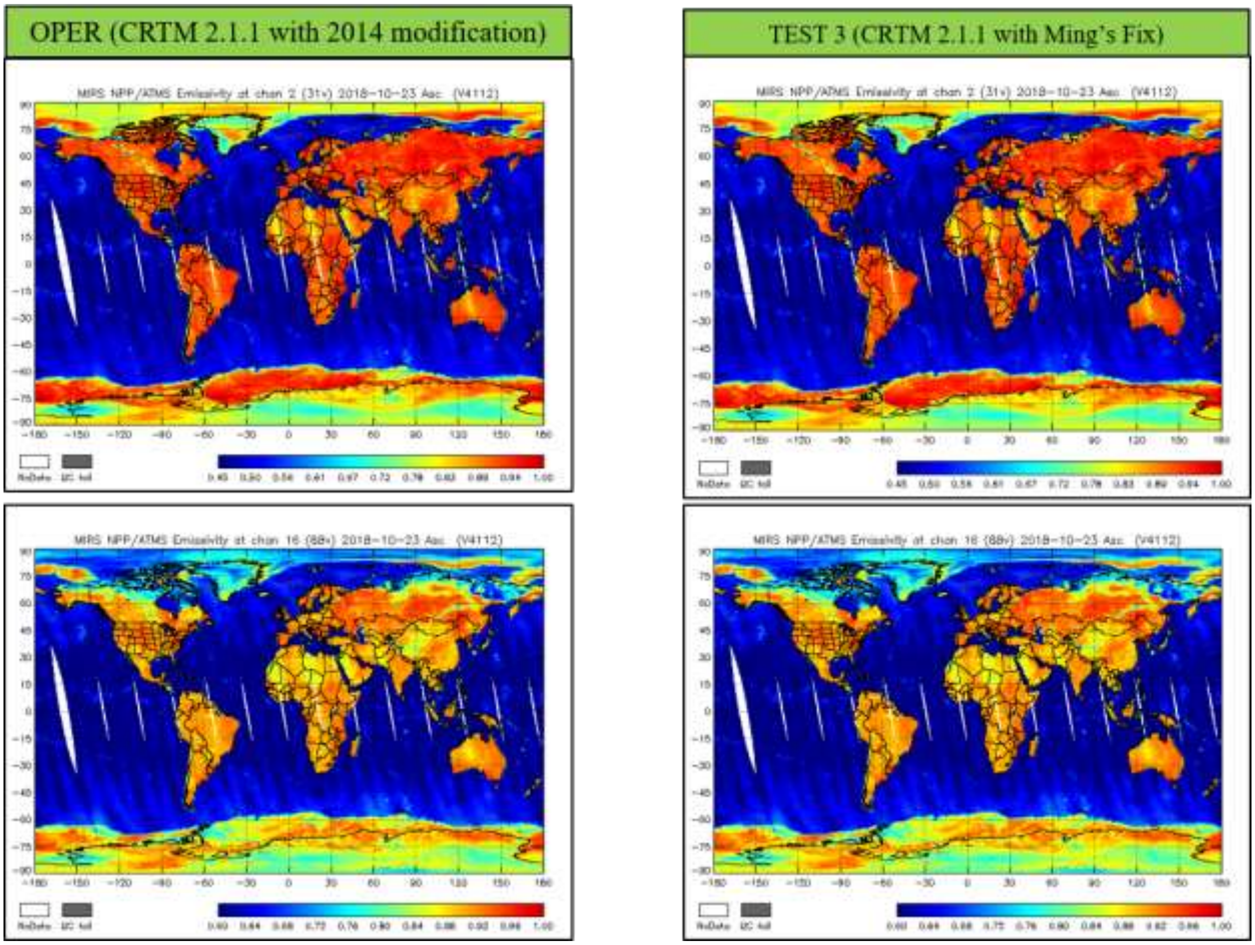


Figure 8. MiRS testing with non-ocean surfaces assumed to be diffusive

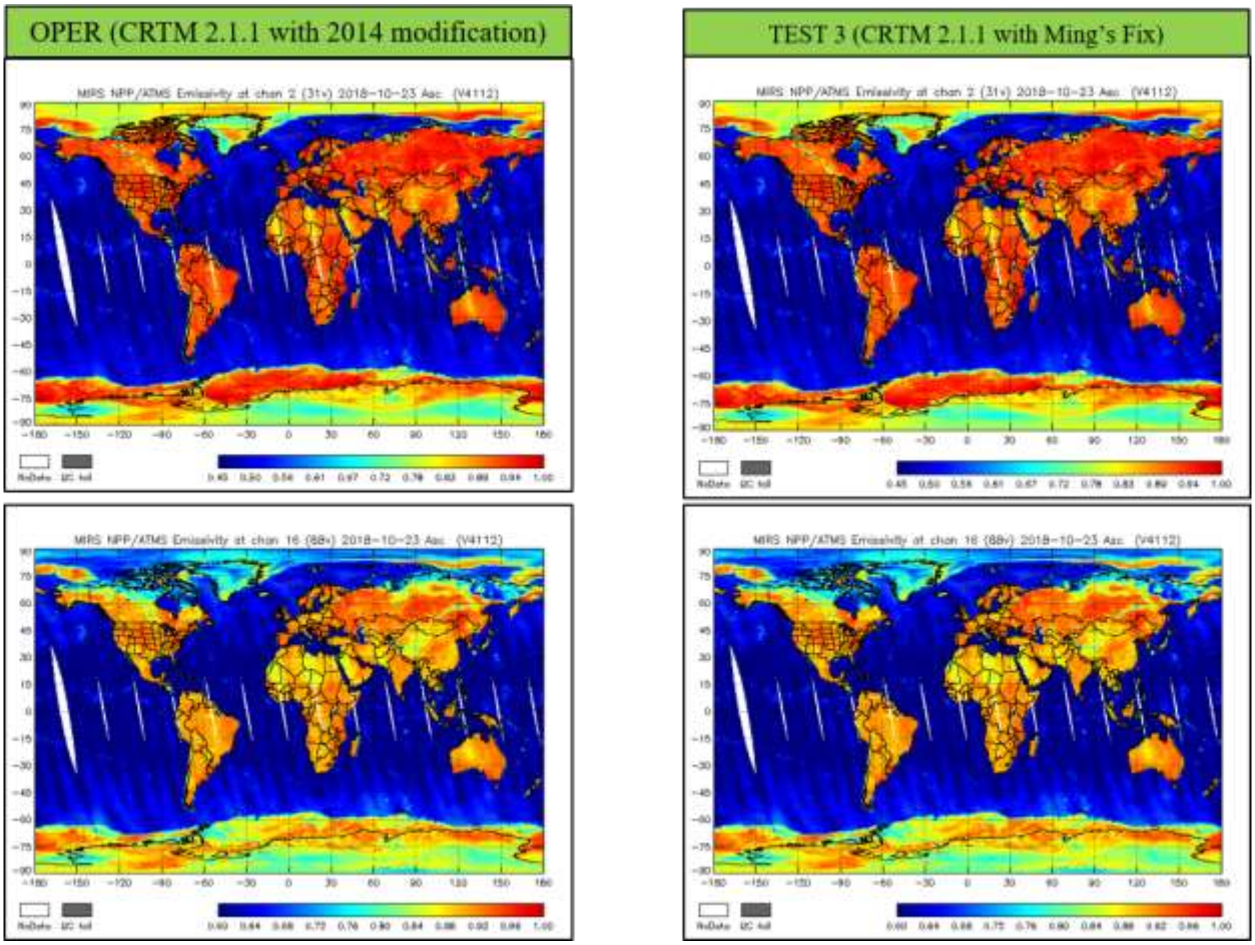


Figure 9. MiRS testing with all surfaces assumed to be specular